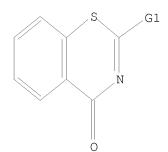
10/537,520 Page 4

STR

=> d l1 L1 HAS NO ANSWERS L1 S'



G1 Cb, Ak

Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 09:10:52 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 498 TO ITERATE

100.0% PROCESSED 498 ITERATIONS 14 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 8622 TO 11298 PROJECTED ANSWERS: 56 TO 504

L2 14 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 09:11:01 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 10083 TO ITERATE

100.0% PROCESSED 10083 ITERATIONS 219 ANSWERS

SEARCH TIME: 00.00.01

L3 219 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST 178.36 178.57

FILE 'CAPLUS' ENTERED AT 09:11:08 ON 13 FEB 2008
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FILE COVERS 1907 - 13 Feb 2008 VOL 148 ISS 7 FILE LAST UPDATED: 12 Feb 2008 (20080212/ED)

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=> s 13

L4 45 L3

=> d ibib abs hitstr tot

Habte 2/13/2008

Page 6

L4 ANSWER 1 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2007:33207 CAPLUS DOCUMENT NUMBER: 146:131801

TITLE:

146:131801
Optical recording medium and benzo-[e]-[1,3]-thiadiazin-4-one derivative
Ishida, Tsutomu; Miyazato, Masataka; Shiozaki,
Hiroyuki; Ogiso, Akira
Mitsui Chemicals Inc., Japan
Jpn. Kokai Tokkyo Koho, 5lpp.
CODEN: J INVENTOR(S):

PATENT ASSIGNEE(S):

DOCUMENT TYPE: LANGUAGE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE JP 2007001094 PRIORITY APPLN. INFO.: JP 2005-182695 JP 2005-182695 20070111 20050622

OTHER SOURCE(S): MARPAT 146:131801

The material contains ≥ 1 benzo-[e]-[1,3]-thiadiazin-4-one derivative in ≥ 0 f the recording layer. The compound I and II (one of the tautomeric structure) (R1-5, R21-24 = H, halo, nitro, cyano, OH, carbonyl alkyl, aralkyl, aryl, metallocenyl, etc.; Ar = aromatic ring) are

claimed.

med. meterial is recorded and read by 300-900 nm laser beam.

The material is recorded and read by 300-900 nm laser beam.

67433-04-9 918647-38-8 918647-40-2

918647-42-4 918647-45-7 918647-47-9

918647-49-1 918647-95-15 918647-53-7

RL: TEM (Technical or engineered material use); USES (Uses)

(optical recording material containing benzothiazinone compound)

67433-04-9 CAPLUS

4H-1,3-Benzothiazin-4-one, 2-(phenylmethyl)- (CA INDEX NAME)

L4 ANSWER 1 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

918647-38-8 CAPLUS 1H-Indene-1,3(2H)-dione, 2-(4-oxo-4H-1,3-benzothiazin-2-y1)- (CA INDEX

918647-40-2 CAPLUS 1H-Phenalene-1,3(2H)-dione, 2-(4-oxo-4H-1,3-benzothiazin-2-yl)- (CA

NAME)

918647-42-4 CAPLUS

| LH-Benz[f]indene-1,3(2H)-dione, 2-(4-oxo-4H-1,3-benzothiazin-2-yl)- (CA INDEX NAME)

ANSWER 1 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

918647-45-7 CAPLUS
1H-Indene-1,3(2H)-dione, 5-(1,1-dimethylethyl)-2-(4-oxo-4H-1,3-benzothiazin-2-yl)- (CA INDEX NAME)

918647-47-9 CAPLUS 1H-Indene-1,3(2H)-dione, 4-[2-(4-morpholiny1)ethoxy]-2-(4-oxo-4H-1,3-benzothiazin-2-y1)- (CA INDEX NAME)

RN 918647-49-1 CAPLUS CN 1H-Indene-5-carboxamide, N,N-diethyl-2,3-dihydro-1,3-dioxo-2-(4-oxo-4H-1,3-benzothiazin-2-yl)- (CA INDEX NAME)

ANSWER 1 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

RN 918647-51-5 CAPLUS
CN 1H-Indene-1,3(2H)-dione,
5,6-dichloro-4,7-bis(2-ethoxyethoxy)-2-(4-oxo-4H-1,3-benzothiazin-2-yl)- (CA INDEX NAME)

918647-53-7 CAPLUS
4H-1,3-Benzothiazin-4-one, 2-(2-anthracenyl)- (CA INDEX NAME)

L4 ANSWER 2 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2005:1010008 CAPLUS

DOCUMENT NUMBER: 144:390853

ACCESSION NUMBER: 2005:1010008 CAPLUS
DOCUMENT NUMBER: 144:390853
ITITLE: Polyfluorobenzoyl chlorides and isothiocyanates in reactions with CH-reactive benzimidazoles
AUTHOR(S): Nosova, E. V., Lipunova, G. N.; Laeva, A. A.;
Charushin, V. N.
CORPORATE SOURCE: Ural State Technical University, Yekaterinburg, 620002, Russia
SOURCE: Russian Chemical Bulletin (2005), 54(3), 733-737
CODEN: RCBUEY; ISSN: 1066-5285
PUBLISHER: Springer Science+Business Media, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: Emglish
CTHER SOURCE(S): CASREACT 144:390853
AB Reactions of 2-(benzoylmethyl)benzimidazole with tetra- and pentafluorobenzoyl chlorides afford fluorine-containing 6-benzoyl-7H-benzimidazo[3,2-a]quinolones. 2-(Cyanomethyl)- or 2(benzoylmethyl)benzimidazole reacts with tetra(penta)fluorobenzoyl isothiocyanates to give fluorine-containing 1,3-benzothiazinones, which differently behave in reactions with cycloalkylimines.
IT 883241-82-5P
RL: RCT (Reactant), SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of fluorinated benzimidazoquinolones and benzothiazinones by cyclocondensation of CH-reactive benzimidazoles with fluorobenzoyl chlorides or isothiocyanates)
RN 883241-79-0 CAPLUS
CN 4H-1, 3-Benzothiazine-2-acetonitrile, \(\alpha (1,3-dihydro-2H-benzimidazol-2-ylidene) -6, 7, 8-trifluoro-4-oxo- (CA INDEX NAME)

883241-80-3 CAPLUS

4H-1,3-Benzothiazine-2-acetonitrile, α-(1,3-dihydro-2H-benzimidazol-2-ylidene)-5,6,7,8-tetrafluoro-4-oxo- (CA INDEX NAME)

ANSWER 2 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

883241-87-0 CAPLUS
4H-1,3-Benzothiazine-2-acetonitrile, α-(1,3-dihydro-2H-benzimidazol-2-ylidene)-6,8-difluoro-7-(4-morpholinyl)-4-oxo- (CA INDEX NAME)

883241-89-2 CAPLUS

4H-1,3-Benzothiazine-2-acetonitrile, a-(1,3-dihydro-2H-benzimidazol-2-ylidene)-6,8-difluoro-5,7-di-4-morpholinyl-4-oxo- (CA INDEX NAME)

REFERENCE COUNT: THIS

THERE ARE 31 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

ANSWER 2 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

RN 883241-81-4 CAPLUS
CN 4H-1,3-Benzothiazin-4-one,
2-[1-(1,3-dihydro-2H-benzimidazo1-2-ylidene)-2oxo-2-phenylethyl]-6,7,8-trifluoro- (CA INDEX NAME)

RN 883241-82-5 CAPLUS
CN 4H-1,3-Benzothiazin-4-one,
2-[1-(1,3-dihydro-2H-benzimidazol-2-ylidene)-2oxo-2-phenylethyl)-5,6,7,8-tetrafluoro- (CA INDEX NAME)

IT 883241-85-8P 883241-87-0P 883241-89-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of fluorinated benzimidazoquinolones and
benzothiazinones by
cyclocondensation of CH-reactive benzimidazoles with fluorobenzoyl
chlorides or isothiocyanates)
RN 883241-85-8 CAPLUS
CN 4H-1, 3-Benzothiazin-4-one,
2-[1-(1,3-dihydro-2H-benzimidazol-2-ylidene)-2oxo-2-phenylethyl]-6,8-difluoro-5,7-di-4-morpholinyl- (CA INDEX NAME)

L4 ANSWER 3 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2004:568612 CAPLUS DOCUMENT NUMBER: 141:123638

LUS COPYRIGHT 2008 ACS on STN
2004:568612 CAPLUS
141:12363
Preparation of 1,3-benzothiazinones as macrophage
migration inhibitory factor binders and apoptosis
inhibitors, and treatment of diseases with them or
their prodrugs
Kajino, Masahiro; Nakayama, Yutaka; Kimura, Atsuhide
Takeda Chemical Industries, Ltd., Japan
Jpn. Kokai Tokkyo Koho, 55 pp.
CODEN: JYKXAF
Patent
Japanese
1

WO 2003-JP15535

W 20031204

INVENTOR(S):

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

								20040715		APPLICATION NO.									
	JP									JP 2003-406172 WO 2003-JP15535									
	WO					A1	2004072								20031204				
		W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,	
			co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,	GE,	
			GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KR,	KZ,	LC,	LK,	LR,	
			LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,	NZ,	OM,	
			PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	TJ,	TM,	TN,	
			TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW				
		RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	AZ,	
			BY,	KG,	KZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	
			ES,	FI,	FR,	GB,	GR,	HU,	IE,	IT,	LU,	MC,	NL,	PT,	RO,	SE,	SI,	SK,	
			TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	
TG																			
	AU	2003		A1		20040729			AU 2003-289176					20031204					
	EP	1568697			A1	20050831			EP 2003-777247					20031204					
		R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,	
			IE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR,	BG,	CZ,	EE,	HU,	SK		
	US	S 2006052371				A1	20060309				US 2005-537520				20050901				
PRIORITY APPLN. INFO.:											JP 2002-353546					A 20021205			

OTHER SOURCE(S): MARPAT 141:123638

Title compds. I [R1 = halo, OH, NO2, (halo)alkyl, acyl, (un)substituted amino, R2 = (un)substituted branched alkyl, (un)substituted cycloalkyl, (un)substituted condensed homocyclic ring residue, substituted Ph; n = 0-4] or their salts, which have low toxicity (no data), are prepared The

ANSWER 3 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued) compds. or their prodrugs are useful for prophylactic and therapeutic treatment of circulation disorders (e.g. heart failure), bone and joint diseases, infectious diseases, inflammation, and kidney diseases. Thus, 2-[(cyclopropylcarbonyl)thio]benzoic acid was treated with ClCO2Et, NaN3, and Bu3P, and cyclized to give I (Rln = H, R2 = cyclopropyl), which inhibited rat myocardial apoptoris with IC50 value of 0.072 µM. 543696-69-1P 722507-36-0P 722507-32-6P 722507-34-6P 722507-36-0P 722507-32-P 722507-46-P 722507-36-0P 722507-36-P 722507-59-P 722507-59-F 722507-59-F 722507-50-F 722507-50-0P 722507-50-0P 722507-50-0P 722507-50-0P 722507-50-P 722507-50-0P 722507-50-P 722507-50-0P 72

or binders and apoptosis inhibitors for treatment of diseases) 543696-69-1 CAPLUS 4H-1,3-Benzothiazin-4-one, 2-(2-methoxyphenyl)- (CA INDEX NAME)

722507-22-4 CAPLUS 4H-1,3-Benzothiazin-4-one, 2-cyclopropyl- (CA INDEX NAME)

722507-32-6 CAPLUS Acetic acid, [3-(4-oxo-4H-1,3-benzothiazin-2-y1)phenoxy]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

ANSWER 3 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

722507-42-8 CAPLUS 4H-1,3-Benzothiazin-4-one, 2-(3-bromophenyl)- (CA INDEX NAME)

722507-44-0 CAPLUS 4H-1,3-Benzothiazin-4-one, 2-(4-hydroxyphenyl)- (CA INDEX NAME)

722507-46-2 CAPLUS
Acetamide, N-[3-(4-oxo-4H-1,3-benzothiazin-2-yl)phenyl]- (CA INDEX NAME)

722507-48-4 CAPLUS Benzonitrile, 4-(4-0x0-4H-1,3-benzothiazin-2-y1)- (CA INDEX NAME)

722507-50-8 CAPLUS

ANSWER 3 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

722507-34-8 CAPLITS

nzenepropanoic acid, 3-(4-oxo-4H-1,3-benzothiazin-2-y1)- (CA INDEX

722507-36-0 CAPLUS
Benzonitrile, 3-(4-oxo-4H-1,3-benzothiazin-2-yl)- (CA INDEX NAME)

722507-38-2 CAPLUS 4H-1,3-Benzothiazin-4-one, 2-[4-(trifluoromethyl)phenyl]- (CA INDEX CN NAME)

722507-40-6 CAPLUS 4H-1,3-Benzothiazin-4-one, 2-(4-acetylphenyl)- (CA INDEX NAME)

ANSWER 3 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued) Benzamide, N,N-diethyl-4-(4-oxo-4H-1,3-benzothiazin-2-yl)- (CA INDEX

722507-52-0 CAPLUS Acetamide, $N-[4-(4-\infty - 4H-1, 3-benzothiazin-2-yl)phenyl]-$ (CA INDEX NAME)

722507-54-2 CAPLUS

4H-1,3-Benzothiazin-4-one, 2-[1,1'-biphenyl]-4-yl- (CA INDEX NAME)

722507-56-4 CAPLUS 4H-1,3-Benzothiazin-4-one, 2-[2-(trifluoromethy1)pheny1]- (CA INDEX

722507-58-6 CAPLUS 4H-1,3-Benzothiazin-4-one, 2-[3-(trifluoromethyl)phenyl]- (CA INDEX

L4 ANSWER 3 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

 $722507-60-0 \quad CAPLUS \\ \text{Benzoic acid, } 3-(4-oxo-4H-1,3-benzothiazin-2-yl)-, methyl ester \quad (CA$ NAME)

722507-62-2 CAPLUS Phenylalanine, N-benzoyl-3-(4-oxo-4H-1,3-benzothiazin-2-yl)-, methyl ester

(CA INDEX NAME)

IT

722507-66-6P 722507-84-8P 722507-88-2P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of benzothiazinones as macrophage migration inhibitory

binders and apoptosis inhibitors for treatment of diseases)
722507-66-6 CAPLUS
Benzenepropanoic acid, 3-(4-oxo-4H-1,3-benzothiazin-2-y1)-,
1,1-dimethylethyl ester (CA INDEX NAME)

L4 ANSWER 3 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

722507-84-8 CAPLUS 4H-1,3-Benzothiazin-4-one, 2-(4-chloro-2-methylphenyl)- (CA INDEX NAME)

722507-88-2 CAPLUS Benzolc acid, 2-(ethylamino)-4-(4-oxo-4H-1,3-benzothiazin-2-y1)-, methyl ester (CA INDEX NAME)

L4 ANSWER 4 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:805367 CAPLUS
TITLE: 138:221554
Synthesis and structural characterization of 4H-1,3-benzothiazine derivatives
Fodor, Lajos; Bernath, Gabor; Sinkkonen, Jari; Pihlaja, Kalevi
CORPORATE SOURCE: Research Group for Heterocyclic Chemistry of the Hungarian Academy of Sciences, Institute of Pharmaceutical Chemistry, University of Szeged, Szeged, H-6701, Hung.
Journal of Heterocyclic Chemistry (2002), 39(5), 927-931
CODEN: JHTCAD; ISSN: 0022-152X
PUBLISHER: HeteroCorporation
DOCUMENT TYPE: Journal
LANGUAGE: CSSEACT 138:221554
AB The ring-closure reactions of N-arylthiomethylaroylamide derivs. [e.g.

CTHER SOURCE(S): CASREACT 138:221554

AB The ring-closure reactions of N-arylthiomethylaroylamide derivs. [e.g., 4-methoxy-N-[(3-methylphenyl)thio]methyl]benzamide, 4-chloro-N-[(3,4-diethoxy-phenyl)thio]methyl]benzamide, etc.] in the presence of phosphorus oxychloride gave 2-aryl-4H-1,3-benzothiazines. 2-(3-chlorophenyl)-6-methyl-4H-1,3-benzothiazine was reduced with 2n to obtain the corresponding 2,3-dihydro derivative Potassium permanganate oxidation of 2-(4-chlorophenyl)-2,3-diethoxy-4H-1,3-benzothiazines gave the corresponding 4-ones. The reactions of 2-(4-chlorophenyl)-6-methyl-4H-1,3-benzothiazine with substituted acetyl chlorides led to linearly condensed 9-lactams. The structures of the compds. studied were confirmed by 1H and 13C NMR and by their characteristic mass spectrometric fragmentations. Azeto[2,1-b][1,3]benzothiazin-1-one derivs. were also prepared

IT 501067-96-3P 501087-97-4P RL: SPN (Synthetic preparation); FREP (Preparation)

501087-96-3P 501087-97-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and structural characterization of (phenyl)benzothiazine
derivs.)
501087-96-3 CAPLUS
4H-1,3-Benzothiazin-4-one, 2-(4-chlorophenyl)-6,7-diethoxy- (CA INDEX

Office (CA INDEX NAME)

ANSWER 4 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

REFERENCE COUNT:

THERE ARE 17 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

L4 ANSWER 5 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2002:428886 CAPLUS DOCUMENT NUMBER: 137:28319 Heterocyclic poly(ADP-ribose) polymerase (PARP) inhibitors
Melese, Teri; Perkins, Edward L.; Yeh, Elaine; Sun, TITLE: INVENTOR(S): Donxu Iconix Pharmaceuticals, Inc., USA PCT Int. Appl., 37 pp. CODEN: PIXXD2 PATENT ASSIGNEE(S): DOCUMENT TYPE: LANGUAGE: English FAMILY ACC. NUM. COUNT: PATENT INFORMATION: PATENT NO. KIND DATE APPLICATION NO. DATE

WO 2001-US46811

OTHER SOURCE(S): MARPAT 137:28319

L4 ANSWER 6 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:401958 CAPLUS
DOCUMENT NUMBER: 135:22080

TITLE: 135:22080

Novel inhibitors of poly(ADP-ribose) polymerase/PARP1
and PARP2 identified using a cell-based screen in

and PARP2 identified using a cell-based screen in yeast Perkins, Ed; Sun, Dongxu; Nguyen, Allen; Tulac, Suzana; Francesco, Michelle; Tavana, Homa; Nguyen, Hieu; Tugendreich, Stuart; Barthmaier, Peter; Couto, Joe; Yeh, Elaine; Thode, Silke; Jarnagin, Kurt; Jain, Ajay; Morgans, David; Melese, Teri Iconix Pharmaceuticals, Mountain View, CA, 94043, USA Cancer Research (2001), 61(10), 4175-4183 CODEN: CNEAB; ISSN: 0008-5472 American Association for Cancer Research Journal AUTHOR(S):

CORPORATE SOURCE: SOURCE:

COEN: CNERAS; ISSN: 0008-5472

PUBLISHER: American Association for Cancer Research
DOCUMENT TYPE: Journal

LANGUAGE: English

Multicellular organisms must have means of preserving their genomic
integrity or face catastrophic consequences such as uncontrolled cell
proliferation or massive cell death. One response is a modification of
nuclear proteins by the addition and removal of polymers of ADP-ribose

modulate the properties of DNA-binding proteins involved in DNA repair and

metabolism These ADP-ribose units are added by poly(ADP-ribose)

metabolism These Australiance and Parameter and Parameter (PARP) and removed by poly(ADP-ribose) glycohydrolase. Although budding yeast Saccharomyces cerevisiae does not possess proteins with significant sequence similarity to the human PARP family of proteins, we identified novel small mol. inhibitors against two family members, PARPI and PARP2, using a cell-based assay in yeast. The assay was based on the reversal

growth inhibition caused by the heterologous expression of either PARP1

 ${\tt PARP2.}$ Validation of the assay was achieved by showing that the growth inhibition was relieved by a mutation in a single residue in the

innibition was carried at a known PARP1 inhibitor, 6(5H)-phenanthridinone. In sep. expts., when a putative protein

lator
of PARP activity, human poly(ADP-ribose) glycohydrolase, was coexpressed
with PARPI or PARP2, yeast growth was restored. Finally, the inhibitors
identified by screening the yeast assay are active in a mammalian PARP
biochem. assay and inhibit PARPI and PARP2 activity in yeast cell exts.
Thus, our data reflect the strength of using yeast to identify small mol.
inhibitors of therapeutically relevant gene families, including those

are not found in yeast, such as PARP. The resultant inhibitors have two critical uses (a) as leads for drug development and (b) as tools to dissect cellular function.

IT 67433-05-0
R.: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified). PTOL (Pir.)

L4 ANSWER 5 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

$$\mathbb{R}^{6} \xrightarrow{\mathbb{R}^{7}} \mathbb{R}^{1} \mathbb{R}^{2} \qquad \mathbb{R}^{13} \xrightarrow{\mathbb{N}} \mathbb{R}^{10} \mathbb{R}^{10}$$

AB Compds. I, II, and III [A1 = C(R4), N; A2 = C(R5), S; R1 = H, lower alkyl,

l, halo, carbonyl; R2 = H, lower alkyl, acyl, or forms double bond with adjacent ring atom; R3 = H, lower alkyl, halo, aryl, etc.; R4 = H, lower alkyl, or forms double bond with adjacent ring atom; R5 = H, lower alkyl, OH, halo, lower alkoxy, etc.; R6, R7 = H, lower alkyl, OH, lower alkoxy, halo, nitro, etc.; R10 = H, lower alkyl, lower alkenyl, aryl, heterocyclyl, etc.; R11=R13 = halo, nitro, OH, NH2, lower alkyl, and pharmaceutically acceptable salts thereof, are effective modulators of

pharmaceutically acceptable saits thereof, are effective modular PARP enzymes. 67433-05-0, ICX 56259537 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (Heterocyclic poly (ADP-ribose) polymerase (PARP) inhibitors) 67433-05-0 CAPLUS 4H-1,3-Benzothiazine-2-acetamide, 4-oxo- (CA INDEX NAME)

ANSWER 6 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

REFERENCE COUNT: THERE ARE 55 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

Page 11

L4 ANSWER 7 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2000:822981 CAPLUS DOCUMENT NUMBER: 133:367807
Silver halide color photographic material containing color developer and coupler and image formation Uchida, Osamu; Ishiwata, Yasuhiro; Katsumata, Taiji Fuji Photo Film Co., Ltd., Japan Jpn. Kokai Tokkyo Koho, 46 pp. CODEN: JKXXAF Fatent 133:367807 TITLE: INVENTOR(S): PATENT ASSIGNEE(S): SOURCE: DOCUMENT TYPE: DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: PATENT NO. KIND DATE APPLICATION NO. DATE 20001124 1999050

JP 2000321733 PRIORITY APPLN. INFO.: JP 1999-127300 JP 1999-127300 OTHER SOURCE(S): MARPAT 133:367807

The material comprises a support having thereon ≥ 1 hydrophilic colloid layer containing ≥ 1 color developer I (C α = C; Z = carbamoyl, acyl, alkowycarbonyl, aryloxycarbonyl, Q = atoms required to form an unsatd. ring with C α 0 and ≥ 1 coupler II (C β = C; EWG = CN, carbamoyl, alkoxycarbonyl; LG = releasing group by coupling-reaction with developer oxidation product; M = atoms required to form 6-membered aromatic heterocyclic ring with C β 1. Images are formed by (1) heat-developing the material; (2) developing it in the presence of alkali generated by slightly soluble metal salt and its complexing it; or agent;

) or (3) developing it with an alkaline developer. The material shows

oved color development, providing images with improved light, heat, and humidity stability.

307496-50-0

RL: DEV (Device component use); USES (Uses)

(photog. film containing developer and coupler)

L4 ANSWER 8 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2000:822980 CAPLUS
DOCUMENT NUMBER: 133:367806
Silver halide color photographic material containing specific coupler and image formation using same
Uchida, Osamu; Ishiwata, Yasuhiro; Katsumata, Taiji
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Uchida, Osamu; Ishiwata, Taiji
PATENT INFORMATION: Japan
ADALENT LOROMATION: Japan
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

JP 2000321732 PRIORITY APPLN. INFO.: 1999050 20001124

OTHER SOURCE(S): MARPAT 133:367806

The title photog, material contains ≥ 1 coupler of the formula I (C β = C atom; EWG = CN, carbamoyl, alkoxycarbonyl; M = atoms required to form an aromatic heterocycle along with C β ; LG = arylthio) in ≥ 1 of the hydrophilic colloid layers formed on a support. The material is heat-developed or developed under such a condition that it alkali

is generated by a slightly soluble metal salt and its complex-forming

or by developing an alkaline processing solution to form images. The lers'
show high coloring properties and stability and provides high quality
color images with high sharpness and storage stability.
307932-98-5
RL: DEV (Device component use); USES (Uses)
(photog. coupler having arylthio group)
307932-98-5
CAPLUS
Acetamide, N-[2-[cyano(4-oxo-7-pentadecy1-4H-1,3-benzothiazin-2yl)methyl]thio]phenyl]-N-methyl- (CA INDEX NAME)

(Continued)

ANSWER 7 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Co: 307496-50-0 CAPLUS Hexadecanamide, N-[2-[[cyano(4-oxo-4H-1,3-benzothiazin-2-y1)methyl]thio]phenyl]-N-methyl- (CA INDEX NAME)

L4 ANSWER 8 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

Page 12

L4 ANSWER 9 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2000:270189 CAPLUS DOCUMENT NUMBER: 133:59023

TITLE:

133:59023 Activated nitriles in heterocyclic synthesis: facile synthesis of heteroarylthymine analogs and their nucleosides Allam, Yehia A.; Chabaka, Laila M.; Nawwar, Galal A. AUTHOR(S):

CORPORATE SOURCE: Pesticide Laboratory, National Research Centre,

Cairo,

Egypt

SOURCE: Heteroatom Chemistry (2000), 11(3), 209-212

COODEN: HETCE8; ISSN: 1042-7163

PUBLISHER: John Wiley & Sons, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

CTHER SOURCE(S): CASRECT 133:59023

AB 5-Heteroarylthymine analogs were synthesized via binucleophilic attack

with bidentate thiols on the cyano group of cyanoacetylurea to form the
heteroarylurea derivs. followed by their cyclization with formamide.

Also, their nucleosides with 2,3,4,6-tetra-O-acetyl-Q-Dglucopytanose were prepared

IT 277754-11-7

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(synthesis of heteroarylthymine analogs and their nucleosides using
activated nitriles)

RN 277754-11-7 CAPLUS

CN 4H-1,3-Benzothiazine-2-acetamide, N-(aminocarbonyl)-4-oxo- (CA INDEX
NAME)

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR

RECORD, ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 10 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN

(Continued)

ANSWER 10 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN SSION NUMBER: 1993:522687 CAPLUS

DOCUMENT NUMBER: 119:122687

Threshold composition of iron-cobalt alloys during TITLE:

their corrosion in inhibited sulfuric acid media Grigor'ev, V. P.; Gershanova, I. M.; Kravchenko, V. AUTHOR(S):

Rostov. Gos. Univ., Rostov., Russia Zashchita Metallov (1992), 28(5), 833-6 CODEN: ZAMEA9; ISSN: 0044-1856 Journal CORPORATE SOURCE:

DOCUMENT TYPE:

LANGGAGE: Russian
AB Weight loss and electrochem. studies were conducted on Fe-(8-69.3)
atomic% Co
alloys in 0.5 M H2SO4 solns. containing 0.05-0.5 mM 2-phenyl-4-oxo-1,3benzothiazine perchlorate (I). Alloys containing less than 18-23
atomic% Co
behave more like Fe and those above the threshold composition have

parameters approaching Co. The I adsorption on the alloys is described

the Freundlich isotherm. 97189-42-9 RL: PROC (Process) (corrosion inhibition by, of iron-cobalt alloys in sulfuric acid

solns.) 97109-42-9 CAPLUS 4H-1,3-Benzothiazin-4-one, 2-phenyl-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 7601-90-3 CMF C1 H O4

CM 2

CRN 7474-08-0 CMF C14 H9 N O S

ACCESSION NUMBER: DOCUMENT NUMBER: TITLE:

ANSWER 11 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN
SSION NUMBER: 1993:416999 CAPLUS
MENT NUMBER: 119:16999
E: Threshold composition of iron-cobalt alloy as a function of solution temperature
OR(S): Grigor'ev, V. P.; Gershanova, I. M.; Kravchenko, V.

AUTHOR(S):

M.

CORPORATE SOURCE:

Rostov. Gos. Univ., Rostov, Russia

SOURCE:

Elektrokhimiya (1993), 29(2), 273-5

CODEN: ELKRAX; ISSN: 0424-8570

DOCUMENT TYPE:

Journal

LANGUAGE:

Russian

AB The influence of the temperature on the threshold composition of an

Fe-Co alloy in

inhibited H2S04 solns. was studied. Fotentiostatic and photocolorimetric methods were used to study the anodic dissoln. of cast Fe-Co alloys (cCo

1.7-69.3 mol.%) in 0.5M H2SO4 containing 1 + 10-4M 2-phenyl-4-oxo-1,3-benzothiazinium perchlorate at temps. of 25-40° in the active range of potentials E (-0.25 to 0.05 V). The reference electrode was saturated Ag chloride.

CM 1

Orlow 197189-42-9 (Properties)
(anodic dissoln. of cobalt-iron alloys in sulfuric acid containing)
97189-42-9 CAPUS
4H-1,3-Bepothiazin-4-one, 2-phenyl-, perchlorate (9CI) (CA INDEX NAME)

CRN 7601-90-3 CMF C1 H O4

CM 2

CRN 7474-08-0 CMF C14 H9 N O S

Page 13

L4 ANSWER 12 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1992:600467 CAPLUS

DOCUMENT NUMBER: 117:200467
TITLE: Threshold concentration of binary iron-cobalt alloys during their anodic dissolution in the presence of surfactants

AUTHOR(S): Grigor'ev, V. P.; Kravchenko, V. M.; Gershanova, I. M.; Aksenova, N. G.

CORPORATE SOURCE: Rostov. Gos. Univ., Rostov, Russia
SOURCE: Zashchita Metallov (1992), 28(3), 390-4
CODEN: ZAMEA9; ISSN: 0044-1856

DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB In the presence of surfactants at a predetd. alloy composition, it is possible
to transfer the control of its dissoln. from 1 component to the other, using Fe-Co alloys as an example. Thus, the anodic dissoln. characteristics were studied of cast Fe-Co alloy in pure and inhibited solns. of H2S04. The Fe-Co alloys contained 1.8, 7.9, 18.8, 24.7, 32.7, 40.2, and 70.8 weight% Co as solid solns. For comparison, samples of Armoo 40.2, and 70.8 weight% Co as solid solns. For comparison, samples of Armco

Fe and Co of grade "K-O" were tested in 0.5M H2SO4 at E (in the active region) of -0.2 to +0.05 V/vs. a normal H electrode. The surfactant additive which was used was 2-phenyl-4-oxo-1,3-benzothiazinium perchlorate. The introduction into the solution of the surfactant, changing

(in different ways) the angular coeffs. of the anodic curves log j vs. E for Co and Fe, lead to the appearance of a threshold composition of the Fe-Co alloy, at which control of the dissoln. kinetics of the alloy passes from 1 compound to the other. 97189-42-9, 2-Phenyl-4-oxo-1,3-benzothiazinium perchlorate RL: PRP (Properties) (anodic dissoln. of iron-cobalt alloys in presence of, threshold concentration entration
of binary alloys in relation to)
97189-42-9 CAPLUS
4H-1,3-Benzothiazin-4-one, 2-phenyl-, perchlorate (9CI) (CA INDEX NAME) CM 1 CRN 7601-90-3 CMF Cl H O4 CM 2

ANSWER 12 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN CRN 7474-08-0 CMF C14 H9 N O S (Continued)

ANSWER 13 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN
SSION NUMBER: 1992:214422 CAPLUS
Licitation of 4-oxo-1,3-benzothiazinium salts.
Synthesis of o-(mercaptophenyl)-1,2,4-triazoles and their metal chelates
OR(S): Ryabukhin, Yu. 1.; Norzhavina, O. B.; Garnovskii, A.
D.; Knyazev, A. P.; Terent'ev, P. B.
ORATE SOURCE: Nauchno-Issed. Inst. Fiz. Org. Khim., Rostov-on-Don, 344090, USSR
Khimiya Geterotsiklicheskikh Soedinenii (1991), (9), 1220-6 ACCESSION NUMBER: DOCUMENT NUMBER: TITLE: AUTHOR(S): CORPORATE SOURCE: 1220-6 CODEN: KGSSAQ; ISSN: 0453-8234 Journal Russian CASREACT 116:214422 DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S): GI

AB 5-(o-Mercaptophenyl)-1,2,4-triazoles I (R = Ph, R1 = H, Ph, PhCH2; R = PhCH2, p-02MCGH4, R1 = Ph) were prepared (50-80% yields) by recyclization of clization of 4-oxo-1,3-benzothiadiazinium perchlorates II with RINHNH2 in refluxing AcOH. Treating I in a min. volume of MeOH with M(OAO)2 (M = Co, Ni, Zn) gave 53-84% complexes III (RI = Ph, M = Co, Ni, Zn, RI = PhCH2, M = Co, Ni). 37103-42-7 RE: RCT (Reactant); RACT (Reactant or reagent) (recyclization of, by hydrazines) 97189-42-9 CAPLUS 4H-1,3-Benzothiazin-4-one, 2-phenyl-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 7601-90-3 CMF C1 H O4

7474-08-0 C14 H9 N O S 97189-44-1 140455-64-7
RL: RCT (Reactant); RRCT (Reactant or reagent)
 (recyclization of, by phenylhydrazine)
97189-44-1 (CRPUS
4H-1,3-Benzothiazin-4-one, 2-(phenylmethyl)-, perchlorate (9CI) (CA IT INDEX NAME) CM 1 CRN 67433-04-9 CMF C15 H11 N O S CM 2 CRN 7601-90-3 CMF C1 H O4

L4 ANSWER 13 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN

(Continued)

Page 14

L4 ANSWER 13 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

140455-64-7 CAPLUS

4H-1,3-Benzothiazin-4-one, 2-(4-nitrophenyl)-, monoperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 106274-04-8 CMF C14 H8 N2 O3 S

ANSWER 14 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

ANSWER 14 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN ESSION NUMBER: 1992:184536 CAPLUS

ACCESSION NUMBER:

DOCUMENT NUMBER: 116:184536

Silver halide photographic material with good storage TITLE: Silver halide photographic material with good st stability Ishiguro, Seiji; Shishido, Tadao; Meguro, Kanji Fuji Photo Film Co., Ltd., Japan Jpn. Kokai Tokkyo Koho, 16 pp. CODEN: JKXXAF Patent

INVENTOR(S):

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE JP 03229241 PRIORITY APPLN. INFO.: 19911011 JP 1990-24227 JP 1990-24227 19900202

The title material contains benzothiazinone I [R1 = (substituted) alkyl, aryl; R2-5 = H, halo, OH, (substituted) alkyl, alkozy, amino, acylamide, sulfonamide, carbamoyl, sulfonamyl, carboxyl, sulfonyl, carboxylate, sulfonate; R2 and R3, R3 and R4, and R4 and R5 may form 5- or 6-membered ring; 1 in the emulsion or other hydrophilic colloid layers. 7474-08-0 140429-89-6

7474-08-0 140429-89-6
RI: TEM (Technical or engineered material use); USES (Uses)
(photog. material containing, for storage stability)
7474-08-0 CAPLUS
4H-1,3-Benzothiazin-4-one, 2-phenyl- (CA INDEX NAME)

140429-89-6 CAPLUS
Benzoic acid, 4-(4-oxo-4H-1,3-benzothiazin-2-yl)-, methyl ester (CA

L4 ANSWER 15 OF ACCESSION NUMBER: DOCUMENT NUMBER: TITLE: Formation

ANSWER 15 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN
SSION NUMBER: 1992:93722 CAPLUS
MENTY NUMBER: 116:93722
E: Electroreduction of organic compounds. 19.

Formation

of benzoanellated sulfur heterocycles by intramolecular cathodic cyclization of dithiocarboxylic esters

AUTHOR(S): Gade, Thomas; Streek, Michael; Voss, Juergen
CORPORATE SOURCE: Inst. Org. Chem., Univ. Hamburg, Hamburg, D-2000/13, Germany
SOURCE: Chemische Berichte (1992), 125(1), 127-41
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German
CTHER SOURCE(S): CASKEACT 116:93722
AB Cathodic reduction of aryl and benzyl dithiopivaloates and related dithioesters with leaving groups at the benzene ring or a side chain yield

the sulfur heterocycles. The product depended on the nature of the starting material and the reaction conditions. In the case of \$\alpha\$-coordithioester, thioindigo is formed. The thioamides show a strong tendency to reductive dehalogenation but the S,N-heterocycles are also formed in minor amts. The formation of the rearranged products is discussed in terms of C,S-splitting in the primarily formed radical anion and subsequent C,C-coupling of the fragments and follow-up reactions.

137092-58-1P
FKL: FKEP (Freparation)
 (preparation of, electrochem.)

137092-58-1 CAPLUS

4H-1,3-Benzothiazin-4-one, 2-(1,1-dimethylethyl)- (CA INDEX NAME)

ACCESSION NUMBER:

DOCUMENT NUMBER:

TITLE:

ANSWER 16 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN

USSION NUMBER: 1992:21013 CAPLUS

INMENT NUMBER: 116:21013

A new recyclization of 1,3-heterocyclic cations to benzimidazolium and perimidinium cations

Vedernikova, I. V.; Konstantinchenko, A. A.;

Ryabukhin, Yu. I.

PORRATE SOURCE: Inst. Org. Phys., Univ. Rostov, Rostov-on-Don, AUTHOR(S):

CORPORATE SOURCE: 344113,

SOURCE . Bulletin des Societes Chimiques Belges (1991),

100(2),

175-81
CODEN: BSCBAG; ISSN: 0037-9646

DOCUMENT TYPE: Journal
LANGUAGE: French
OTHER SOURCE(S): CASREACT 116:21013

AB Reaction of 1,3-heterocyclic cations, such as benzoxazinonium,
benzothiazolium, or dithiolanium cations, with o-phenylenediamines or
1,8-maphthalenediamines gave benzimidazolium and perimidinium cations.

IT 97189-42-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with phenylenediamines and naphthalenediamines)
RN 97189-42-9 CAPLUS
CN 4B-1,3-Benzothiazin-4-one, 2-phenyl-, perchlorate (9CI) (CA INDEX NAME)

CRN 7601-90-3 CMF C1 H O4

CM 2

CRN 7474-08-0 CMF C14 H9 N O S

L4 ANSWER 17 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1990:215913 CAPLUS
DOCUMENT NUMBER: 112:215913
Ring-transformation reactions of 1,3-benzothiazines.
Part 5. Saturated heterocycles. Part 140. Synthesis

benzisothiazoles by the oxidative ring contraction of 2-aryl-4H- and 4-aryl-2H-1,3-benzothiazines Szabo, Janos; Szucs, Erzsebet; Fodor, Lajos; Katocs, Agnes; Beznath, Gabo: Oyodyszereszi Vegytani Intez., Szent-Gyorgi Albert Orvostudo. Egyet., Szeged, 6701, Hung.
Magyar Keniai Folyoirat (1989), 95(11), 455-61 CODEN: MSKFA3; ISSN: 0025-0155
Journal Hungarian CASREACT 112:215913

AUTHOR(S):

CORPORATE SOURCE:

DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S): GI

Habte

Dimethoxyphenylbenzothiazine (I) was oxidized with H2O2 to yield the disulfide (II). KMnO4 oxidation of I gave benzothiazin-4-one (III) (R = CMe); which was oxidized with calculated amts. of perbenzoic acid to increase of the contract of

Obtain the corresponding 1-oxide and 1,1-dioxide. Oxidation of III (R = MeO,

Eto,

H) with NaIO4 involved ring contraction, yielding benzisothiazolone
1-oxides (IV). A similar ring transformation was observed in the
oxidation of
aryl benzothiazines (V) (R = alkoxy, Ar = substituted Ph), resulting in
the formation of aryldialkoxybenzisothiazoles (VI). The mechanism of
these ring transformations is discussed.

L4 ANSWER 16 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

ANSWER 17 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued) 117999-13-0
RL: PRP (Properties)
(intermediacy of, in oxidative ring closure of arylbenzothiazine derivative)
117999-13-0 CAPLUS
4H-1,3-Benzothiazin-4-one, 6,7-diethoxy-2-phenyl-, 1-oxide (CA INDEX NAME)

IT

7474-08-0 101734-42-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidative ring contraction of, with sodium periodate)
7474-08-0 CAPLUS
4H-1,3-Benzothiazin-4-one, 2-phenyl- (CA INDEX NAME)

101734-42-3 CAPLUS 4H-1,3-Benzothiazin-4-one, 6,7-diethoxy-2-phenyl- (CA INDEX NAME)

117999-12-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and hydrogenation/ring-contraction sequence of)
117999-12-9 CAPLUS
4H-1,3-Benzothiazin-4-one, 6,7-dimethoxy-2-phenyl-, 1-oxide (CA INDEX NAME)

2/13/2008

Page 16

L4 ANSWER 17 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

IT 56755-15-8P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and oxidation and oxidative ring contraction of, with sodium

periodate) 56755-15-8 CAPLUS

56755-15-8 CAPLUS 4H-1,3-Benzothiazin-4-one, 6,7-dimethoxy-2-phenyl- (CA INDEX NAME)

IT

11/99-14-1P RE: SPN (Synthetic preparation); PREP (Preparation) (preparation of) 11799-14-1 CAPLUS 4H-1,3-Benzothiazin-4-one, 6,7-dimethoxy-2-phenyl-, 1,1-dioxide (CA CN 4.. INDEX NAME)

ANSWER 18 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

ANSWER 18 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN SSION NUMBER: 1989:135187 CAPLUS

DOCUMENT NUMBER: TITLE:

1909:135187 CAPLUS
110:135187 CAPLUS
110:135187

AUTHOR(S):

CORPORATE SOURCE:

DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S): GI

Cyclocondensation of C13CC(NH2)=CRCN (R = C02Et, Bz) with 1,2-R1C6H4R2

(R1

NH2, R2 = NH2, OH; R1 = SH, NH2, R2 = CO2H) or HSCH2CO2H gave heterocycles I (X = NH, O) and II (X = S, NH) and thiazole III, resp. 119707-18-5P 119707-23-2P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) 119707-18-5 CAPLUS 4H-1, 3-Benzothiazine-2-acetic acid, α-cyano-4-oxo-, ethyl ester (CA INDEX NAME)

119707-23-2 CAPLUS 4H-1,3-Benzothiazine-2-acetonitrile, $\alpha\text{-}\text{benzoyl-4-oxo-}$ (CA INDEX NAME)

ACCESSION NUMBER: DOCUMENT NUMBER:

ANSWER 19 OF 45 CAPLUS COPYRIGHT 2008 ACS ON STN

SSION NUMBER: 1989;38956 CAPLUS

MENT NUMBER: 110:38956

Inc: Nitriles in heterocyclic synthesis:
1-cyanoformanilide as precursor for a variety of heterocyclic ring systems

SOR(S): Sherif Mourad; Mohareb, Fafaat Milad; Elgemeie, Galal Eldin H; Singh, Rajendra Prasad

ORATE SOURCE: Galal Country, Giza, Egypt

Heterocycles (1980), 27(7), 1579-83

CODEN: HTCYAM, ISSN: 0385-5414

JOURNAL SOURCE(S): CASREACT 110:38956

AUTHOR(S):

CORPORATE SOURCE:

DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S): GI

PhNHCOCN (I) was converted to quinoxaline derivative II and other

heterocycles III (ZI = O, NH). I was treated with o-phenylenediamine in DMF

III (Z1 = O, NH). I was treated with o-phenylehedramine in All containing piperidine to give II. III (Z1 = O) was prepared from I, salicylic acid, and Et3N in EtOH. Pyrrolinone IV was obtained from I and CH2(CN)2.

IT 118372-86-4P

RI: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)
118372-86-4 CAPLUS
48-1,3-Benzothiazine-2-carboxamide, 4-oxo-N-phenyl- (CA INDEX NAME)

Page 17

ANSWER 20 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER:

DOCUMENT NUMBER:

TITLE:

1989:8142 CAPLUS
110:8142
Ring transformations of 1,3-benzothiazines. 5.
Synthesis of benzisothiazoles by the oxidative ring
contraction of 2-aryl-4H- and 4-aryl-2H-1,3benzothiazines
Szabo, Janos; Szucs, Erzsebet; Fodor, Lajos; Katocs,
Agmes; Bernath, Gabor; Sohar, Pal
Inst. Pharm. Chem., Albert Szent-Gyorgyi Med. Univ.,
Szeged, H-6701, Hung.
Tetrahedron (1938), 44(10), 2985-92
CODEN: TETRAB; ISSN: 0040-4020
Journal
English
CASREACT 110:8142

AUTHOR(S): CORPORATE SOURCE:

SOURCE.

DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S): GI

AB 4H-1,3-Benzothiazine I was oxidized with H2O2 to give disulfide II, whereas the oxidation of I with RMnO4 gave 4H-1,3-benzothiazine-4-one III (R

OMe) (IV). Oxidation of IV with calculated amts. of perbenzoic acid gave the

the corresponding 1-oxide and 1,1-dioxide. III (R = CMe, H, OEt) were oxidized with NaIO4 to give 1,2-benzisothiazol-3(2H)-ones V (R = same). 2H-1,3-Benzothiazines VI [R1 = CMe, R2 = Ph, C6H4Me-4, C6H4Cl-2,

C6H4Cl-4,
C6H3(CMe)2-3,4', R1 = OEt, R2 = Ph] were oxidized with NaIO4 to give the corresponding 1,2-benzisothiazoles VII.
IT 7474-08-0 101734-42-3

ANSWER 20 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

117999-13-0P 117999-14-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
117999-13-0 CAPLUS
4H-1,3-Benzothiazin-4-one, 6,7-diethoxy-2-phenyl-, 1-oxide (CA INDEX NAME)

117999-14-1 CAPLUS

4H-1,3-Benzothiazin-4-one, 6,7-dimethoxy-2-phenyl-, 1,1-dioxide (CA INDEX

NAME)

ANSWER 20 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN RL: RCT (Reactant); RACT (Reactant or reagent) (oxidative ring contraction of) 7474-08-0 CAPLUS (Continued)

4H-1,3-Benzothiazin-4-one, 2-phenyl- (CA INDEX NAME)

101734-42-3 CAPLUS 4H-1,3-Benzothiazin-4-one, 6,7-diethoxy-2-phenyl- (CA INDEX NAME)

56755-15-8P 117999-12-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and oxidative ring contraction of)
56755-15-8 CAPLUS
4H-1,3-Benzothiazin-4-one, 6,7-dimethoxy-2-phenyl- (CA INDEX NAME)

RN 117999-12-9 CAPLUS

4H-1,3-Benzothiazin-4-one, 6,7-dimethoxy-2-phenyl-, 1-oxide (CA INDEX NAME)

ACCESSION NUMBER: DOCUMENT NUMBER: TITLE:

ANSWER 21 OF 45 CAPLUS COPYRIGHT 2008 ACS ON STN
SSION NUMBER: 1987:515548 CAPLUS
MENT NUMBER: 107:115548
E: Nitriles in heterocyclic synthesis: a route for synthesis of functionally substituted thiazinones
Abed, Nosrat M.; Ibrahim, Nadia S.; Aziz, Suzan I.
CRATE SOURCE: Chem. Dep., Fac. Sci., Giza, Egypt
CCE: Revista Portuguesa de Quimica (1985), 27(3-4), 459-62
CODEN: RPTQAT; ISSN: 0035-0419
UMGE: English
R SOURCE(S): CASREACT 107:115548 AUTHOR (S):

CORPORATE SOURCE: SOURCE:

DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S): GI

1,3-Benzothiazines I and II (Z1 = NNHPh, CHPh) were prepared The

reaction
of 2-HSC6H4CO2H with a thiazolineacetonitrile derivative gave I. II (Z1

CHPh) was obtained from 2-HSC6H4CO2H and PhCH:C(CN)2. 67433-0.2-7

6/433-U2-7 (Reactant); RACT (Reactant or reagent) (cycloaddn.-cyclocondensation and condensation reactions of) 67433-02-7 CAPLUS 4H-1,3-Benzothiazine-2-acetonitrile, 4-oxo- (CA INDEX NAME)

107009-63-2P 109419-37-6P 109419-38-7P 109419-39-8P 109419-40-1P 109419-41-2P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) 107009-63-2 CAPLUS 4H-1,3-Benzothiazine-2-acetonitrile, 4-oxo-α-(phenylhydrazono)-(9CI) (CA INDEX NAME)

L4 ANSWER 21 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

109419-37-6 CAPLUS 4H-1,3-Benzothiazin-4-one, 2-[(4,5-dihydro-4-oxo-2-thiazoly1)methy1]-INDEX NAME)

109419-38-7 CAPLUS 4H-1, 3-Benzothiazine-2-acetonitrile, 4-oxo- α -(phenylmethylene)- (CA INDEX NAME)

109419-39-8 CAPLUS 4H-1,3-Benzothiazine-2-acetonitrile, $\alpha\text{-[hydroxy(phenylamino)methylen el-4-oxo-(CA INDEX NAME)}$

L4 ANSWER 21 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

109419-40-1 CAPLUS 4H-1,3-Benzothiazine-2-acetonitrile, α -[mercapto(phenylamino)methyle ne]-4-oxo- (CA INDEX NAME)

109419-41-2 CAPLUS 4H-1,3-Benzothiazine-2-acetonitrile, $\alpha\text{-}(aminohydroxymethylene)-4-oxo-(CA INDEX NAME)}$

L4 ANSWER 22 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1987:458953 CAPLUS
DOCUMENT NUMBER: 107:58953

AUTHOR(S):
AUTHOR(S):
CORPORATE SOURCE: Source: Moustafa Abed, Nosrat; Ibrahim, Nadia Sobhi
Fac. Sci., Cairo Univ., Giza, Egypt
Journal of the Chemical Society of Pakistan (1986), 8(3), 319-22
CODEN: JCSPDF; ISSN: 0253-5106
DOCUMENT TYPE: Journal
LANGUAGE: CASREACT 107:58953
GI

DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S): GI

The reaction of thiosalicylic acid with a variety of activated nitriles

described. Several new benzo[e]-1,3-thiazinones, e.g. I and II are

described. Several new benzo[e]-1,3-thiazinones, e.g. I and II reported. $107009-63-2P\ 109419-37-6P\ 109419-38-7P\ 109419-40-1P\ 109419-41-2P\ RL: SFN (Synthetic preparation); PREP (Preparation) (preparation of) <math display="block">107009-63-2\ CAPLUS\ 4H-1,3-Benzothiazine-2-acetonitrile,\ 4-oxo-\alpha-(phenylhydrazono)-(9CI) (CA INDEX NAME)$ IT

109419-37-6 CAPLUS 4H-1,3-Benzothiazin-4-one, 2-[(4,5-dihydro-4-oxo-2-thiazoly1)methy1]-

INDEX NAME)

ANSWER 22 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

109419-38-7 CAPLUS 4H-1,3-Benzothiazine-2-acetonitrile, 4-oxo- α -(phenylmethylene)- (CA INDEX NAME)

109419-39-8 CAPLUS 4H-1, 3-Benzothiazine-2-acetonitrile, α -[hydroxy(phenylamino)methylen e]-4-oxo- (CA INDEX NAME)

109419-40-1 CAPLUS 4H-1, 3-Benzothiazine-2-acetonitrile, $\alpha\text{-[mercapto(phenylamino)methyle ne]-}4-oxo- (CA INDEX NAME)$

109419-41-2 CAPLUS 4H-1,3-Benzothiazine-2-acetonitrile, $\alpha\text{-}(aminohydroxymethylene)-4-oxo-(CA INDEX NAME)}$

Habte

2/13/2008

L4 ANSWER 22 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

67433-02-7
RL: RCT (Reactant); RACT (Reactant or reagent)
 (reactions of)
67433-02-7 CAPLUS
4H-1,3-Benzothiazine-2-acetonitrile, 4-oxo- (CA INDEX NAME)

ANSWER 23 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued) 4H-1,3-Benzothiazine-2-acetonitrile, $\alpha-[(4-\text{nitrophenyl})\,\text{hydrazono}]$ -4-oxo- (9C1) (CA INDEX NAME)

67433-02-7 107009-64-3 107009-65-4 107009-66-5 107032-75-7 107032-76-8 RL: PROC (Process) (ionization of, in alc. buffered media) 67433-02-7 CAPLUS 4H-1,3-Benzothiarine-2-acetonitrile, 4-oxo- (CA INDEX NAME)

107009-64-3 CAPLUS

4H-1,3-Benzothiazine-2-acetonitrile, α -[(3-chlorophenyl)hydrazono]-4-oxo-(9CI) (CA INDEX NAME)

107009-65-4 CAPLUS 4H-1,3-Benzothiazine-2-acetonitrile, $\alpha-[(3-methylphenyl)hydrazono]-4-oxo-(9C1) (CA INDEX NAME)$

107009-66-5 CAPLUS 4H-1,3-Benzothiazine-2-acetonitrile, α -[(4-methylphenyl)hydrazono]-4-

ANSWER 23 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN ESSION NUMBER: 1987:101585 CAPLUS UMENT NUMBER: 106:101585

ACCESSION NUMBER:

DOCUMENT NUMBER:

Ionization and electroreduction of some TITLE:

benzothiazin-4-one azo dyes Abed, N. M.; Nashed, B.; Fahmy, H. M.; Azzem, M. AUTHOR(S):

Abdel CORPORATE SOURCE: SOURCE:

Fac. Sci., Cairo Univ., Giza, Egypt Monatshefte fuer Chemie (1986), 117(5), 599-605 CODEN: MOCMB7; ISSN: 0026-9247 Journal

DOCUMENT TYPE:

LANGUAGE:

AB The pKa values of benzothiazin-4-ones I (R = H, 3-Cl, 4-Cl, 3-Me, 4-Me, 3-No2, 4-No2) together with a model 2-(cyanomethyl)-4H-3,1-benzothiazin-4-one were determined spectrophotometrically in alc. buffered media. These values were correlated to different o sets. The polarog. behavior of I (R = H, 4-No2) was studied in detail. The obtained data showed that I (R = H) is reduced via a 2-electron process to the corresponding

RN 107009-67-6 CAPLUS

ANSWER 23 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN oxo- (9CI) (CA INDEX NAME) (Continued)

107032-75-7 CAPLUS 4H-1,3-Benzothiazine-2-acetonitrile, $\alpha-[(4-{\rm chlorophenyl})hydrazono]-4-ozo- (9C1) (CA INDEX NAME)$

107032-76-8 CAPLUS

10/032-76-6 CAPLOS 4H-1,3-Benzothiazine-2-acetonitrile, α -[(3-nitrophenyl)hydrazono]-4-oxo-(9CI) (CA INDEX NAME)

(Continued)

(Continued)

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L4 ANSWER 24 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1986;549$60 CAPLUS
DOCUMENT NUMBER: 105:1449$60
CRIGINAL REFERENCE NO: 105:23209a,23212a
TITLE: The new ligand
1,3-diphenyl-5-(o-mercaptophenyl)-1,2,4-
triazole. Freparation and mode of coordination to
metals
AUTHOR(S): Garnovskii, A. D.; Korzhavina, O. B.; Ryabukhin, Yu.
1.

CORPORATE SOURCE: Rostov. Gos. Univ., Rostov, USSR
SOURCE: Rostov. Gos. Univ., Rostov, USSR
SOURCE: Kocholinationaya Khimiya (1986), 12(6), 853-4
CODEN: KOKHOE; ISSN: 0132-344X
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB 1,3-Diphenyl-5-(o-mercaptophenyl)-1,2,4-triazole (HL) was prepared by
bolling in HOAc solution 4-hydroxy. 1,3-benzothiazinium perchlorate and
phenylhydrazine with subsequent treating with H2O. ML2 (M = Co, Ni) were
prepared and characterized by IR spectra. Nil2 is square planar whereas
Col2 is polymeric octahedral. The ligand coordinates through the S and
N(4) atoms. Aerial oxidation of HL gave the corresponding disulfide.

IT 97189-42-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with phenylhydrazine)
RN 97189-42-9 CAPLUS
CM 11
     ACCESSION NUMBER:
                                 CRN 7601-90-3
CMF C1 H O4
                                 CM 2
                                    CRN 7474-08-0
                                    CMF C14 H9 N O S
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L4 ANSWER 24 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN

ANSWER 25 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN

1985:437436 CAPLUS

IMENT TYPE:

UNENT TYPE:

USANGE:

ANSWER 25 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN

1985:437436 CAPLUS

103:37436 CAPLUS

103:6075a,6078a

Synthesis of 4-oxo-1,3-benzothiazines and their salts

Korzhavina, O. B.; Ryabukhin, Yu. I.; Garnovskii, A.
D.; Shavel, I. I.

Rostov. Gos. Univ., Rostov-on-Don, 334077, USSR

Khimiya Geterotsiklicheskikh Soedinenii (1985), (4),
562-3

CODEN: KGSSAQ; ISSN: 0453-8234

JOURNALL SOURCE(S):

CASREACT 103:37436 L4 ANSWER 25 OF 45 CA
ACCESSION NUMBER:
DOCUMENT NUMBER:
ORIGINAL REFERENCE NO.:
TITLE:
AUTHOR(S): CORPORATE SOURCE: DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S): GI

Cyclocondensation of o-HSC6H4CO2H with RCN (R = Ph, PhCH2) in dioxane containing HCl and 70% HClO4-Ac2O gave 60-70% complexes I which were AB

Containing N-1 and N-2 interface gate to the complexes ted with H2O or Et3N to give benzothiazines II; recrystn. of the complexes from AcOH or the action of heat gave 97 and 75% perchlorates III which could also be converted to II. 97189-42-9F 97189-44-IP RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and hydrolysis of) 97189-42-9 CAPLUS 4H-1,3-Benzothiazin-4-one, 2-phenyl-, perchlorate (9CI) (CA INDEX NAME)

CM 1 CRN 7601-90-3 CMF C1 H O4

CM 2 CRN 7474-08-0 CMF C14 H9 N O S 97189-44-1 CAPLUS 4H-1,3-Benzothiazin-4-one, 2-(phenylmethyl)-, perchlorate (9CI) (CA CN 4... INDEX NAME) CM 1 CRN 67433-04-9 CMF C15 H11 N O S

L4 ANSWER 25 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN

CM 2 CRN 7601-90-3 CMF C1 H O4

7474-08-0P 67433-04-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with perchloric acid)
7474-08-0 CAPLUS
4H-1,3-Benzothiazin-4-one, 2-phenyl- (CA INDEX NAME)

L4 ANSWER 25 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

67433-04-9 CAPLUS 4H-1,3-Benzothiazin-4-one, 2-(phenylmethyl)- (CA INDEX NAME)

97189-43-0P 97189-45-2P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation, hydrolysis, and thermal decomposition of) 97189-43-0 CAPLUS 4H-1,3-Benzothiazin-4-one, 2-phenyl-, perchlorate, compd. with

CN 4H-1,3-Benzochil. 1,4-dioxane (2:1) (9CI) (CA INDEX NAME)

CM 1

CRN 123-91-1 CMF C4 H8 O2

CM 2

CRN 97189-42-9 CMF C14 H9 N O S . C1 H O4

CM 3

CRN 7601-90-3 CMF Cl H O4

ANSWER 25 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

CRN 7601-90-3 CMF Cl H O4

L4 ANSWER 25 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

CM 4

CRN 7474-08-0 CMF C14 H9 N O S

97189-45-2 CAPLUS
4H-1,3-Benzothiazin-4-one, 2-(phenylmethyl)-, perchlorate, compd. with
1,4-dioxane (2:1) (9CI) (CA INDEX NAME)

CRN 123-91-1 CMF C4 H8 O2

CM 2

CRN 97189-44-1 CMF C15 H11 N O S . C1 H O4

CM 3

CRN 67433-04-9 CMF C15 H11 N O S

L4 ANSWER 26 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1985:6351 CAPLUS
DOCUMENT NUMBER: 102:6351
CRIGINAL REFERENCE NO: 102:1151a,1154a
TITLE: Nitriles in heterocyclic synthesis: a new approach
for the synthesis of thiazinones
AUTHOR(S): Ibrahim, Nadia S., Abed, Nosrat M., Kandeel, Zaghloul
E.

E. Fac. Sci., Cairo Univ., Giza, Egypt Heterocycles (1984), 22(8), 1677-82 CODEN: HTCYAM; ISSN: 0385-5414 Journal English CASREACT 102:6351 CORPORATE SOURCE:

DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S): GI

The benzothiazinones I (R = cyano, CONH2, CONHPh, CO2Et) were prepared in 60-90% yields by cyclization of o-HSC6H4CO2H with RCH2CN. Reaction of o-HSC6H4CO2H with CL3CCN gave the thiazinone derivative II in 80% yield. 67433-02-79 67433-03-89 RL: RCT (Reactant); SFN (Synthetic preparation); FREP (Preparation); RACT (Reactant or reagent) (preparation and reaction of, with thiosalicylic acid) 67433-02-7 CAPLUS 4H-1,3-Benzothiazine-2-acetonitrile, 4-oxo- (CA INDEX NAME) AB

CH2-CN

67433-03-8 CAPLUS 4H-1,3-Benzothiazine-2-acetic acid, 4-oxo-, ethyl ester (CA INDEX NAME)

Page 22

L4 ANSWER 26 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

67433-05-0P 93666-41-2P 93666-42-3P 93666-44-5P

93606-44-5P
RI: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
67433-05-0 CAPLUS
4H-1,3-Benzothiazine-2-acetamide, 4-oxo- (CA INDEX NAME)

93666-41-2 CAPLUS
4H-1,3-Benzothiazine-2-acetamide, 4-oxo-N-phenyl- (CA INDEX NAME)

93000-42-3 CAPLUS 4H-1,3-Benzothiazin-4-one, 2,3-dihydro-2-[(4-oxo-4H-1,3-benzothiazin-2-yl)methylene]- (CA INDEX NAME)

93666-44-5 CAPLUS 4H-1,3-Benzothiazine-2-ethanethioamide, α -[1-amino-2-(4-oxo-4H-1,3-benzothiazin-2-yl)ethylidene]-4-oxo- (CA INDEX NAME)

ACCESSION NUMBER:
DOCUMENT NUMBER:
ORIGINAL REFERENCE NO.:
TITLE:

AUTHOR(S):

ANSWER 27 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN

DESSION NUMBER: 1982:472312 CAPLUS

JINAL REFERENCE NO:: 97:12105a, 12108a

LE: 1982:472312 CAPLUS

JINAL REFERENCE NO:: 97:12105a, 12108a

Studies of heterocyclic chemistry. Part 25.

Intramolecular cyclizations of N
acylarylethanethioanides leading to thiazoles,

4H-1,3-thlazines, 4H-pyrido[3,2-e]-1,3-thiazines, and

4H-1,3-benzothiazines, 4H-pyrido[3,2-e]-1,3-thiazines, and

4H-1,3-benzothiazines, 4H-pyrido[6,2-e]-1,3-thiazines, and

4H-1,3-benzothiazines, 4H-pyrido[7,2-e]-1,3-thiazines, and

4H-1,3-benzothiazines, 4H-pyrido[7,2-e]-1,3-thiazines

DOCUMENT TYPE:

LANGUAGE: OTHER SOURCE(S): GI English CASREACT 97:72312

AB Cycloaddn. reactions of 4-aryl-3-haloacylthio-, 4-aryl-3-(2-chloronicotinoylthio)-, and
4-aryl-3-(o-halobenzoylthio)-3-isothiazoline-5thiones with acetylenes gave (oxodihydrothiazolylmethylene)-,
(oxodihydrothiazinylmethylene)-, and
(oxopyridothiazinylmethylene) dithiane
s. E.g., refluxing isothiazolinethione I with MeO2CC.tplbond.CCO2Me gave
62% thiazolone II. Intramol. photochem. cyclocondensation reactions of
No-halobenzoyl(1,3-dithiol-2-ylidene) arylethanethioamides gave
oxobenzothiazinylmethylenedithioles. E.g., irradiation of

L4 ANSWER 26 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

ANSWER 27 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued) iodobenzoylthioamide III in THF under N for 10 h gave 67% benzothiazinone

1,3-Dithiole-4,5-dicarboxylic acid, 2-[(4-methylphenyl)(4-oxo-4H-1,3-benzothiazin-2-yl)methylene]-, dimethyl ester (SCI) (CA INDEX NAME)

1,3-Dithiole-4,5-dicarboxylic acid, 2-[(4-chloropheny1)(4-oxo-4H-1,3-benzothiazin-2-yl)methylene]-, dimethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 27 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

78959-07-6 CAPLUS 1,3-Dithiole-4,5-dicarboxylic acid, 2-[(4-methylphenyl)(4-oxo-4H-1,3-benzothiazin-2-yl)methylene]-, diethyl ester (9CI) (CA INDEX NAME)

82491-22-3 CAPLUS 1,3-Dithiole-4,5-dicarboxylic acid, 2-[(4-oxo-4H-1,3-benzothiazin-2-yl)phenylmethylene]-, diethyl ester (9CI) (CA INDEX NAME)

RN 82491-23-4 CAPLUS

ANSWER 27 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued) 4H-1,3-Benzothiazin-4-one, 2-[(4,5-dibenzoyl-1,3-dithiol-2-ylidene)(4-methylphenyl)methyl]- (CA INDEX NAME)

RN 82491-24-5 CAPLUS
CN 1,3-Dithiole-4,5-dicarboxylic acid,
2-[(7-chlor-4-oxo-4H-1,3-benzothiazin2-yl)phenylmethylene]-, dimethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 28 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1981:515430 CAPLUS
DOCUMENT NUMBER: 95:115430
CRIGINAL REFERENCE NO.: 95:19373a,19376a
TITLE: A new and efficient approach to a
4H-1,3-benzothiazine

ring that utilizes the photocyclization of N-o-iodobenzoylthioamides: the ring transformation $% \left(1\right) =\left(1\right) \left(1\right) \left$

AUTHOR(S):

isothiazoles
Nishiwaki, Tarozaemon; Kawamura, Etsuko; Abe,
Noritaka; Sazaoka, Yoshiro; Kochi, Hirafumi
Fac. Sci., Yamaquchi Univ., Yamaquchi, 753, Japan
Heterocycles (1981), 16(7), 1203-4
CODEN: HTCYAM; ISSN: 0385-5414
Journal
English
CASREACT 95:115430

CORPORATE SOURCE:

DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S): GI

II

AB

Irradiation of iodobenzoylthioamides I (R = Me, Et; R1 = Ph, 4-MeC6H4, 4-C1C6H4) in THF gave 83-93% benzothiazinones II.
78959-04-3P 78959-05-4P 78959-06-5P
78959-07-6P
RL: SFN (Synthetic preparation); PREP (Preparation)
(preparation of:
78959-04-3 CAPLUS
1,3-Dithiole-4,5-dicarboxylic acid, 2-[(4-oxo-4H-1,3-benzothiazin-2-yl)phenylmethylene]-, dimethyl ester (9CI) (CA INDEX NAME)

ANSWER 28 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

78959-05-4 CAPLUS 1,3-Dithiole-4,5-dicarboxylic acid, 2-[(4-methylphenyl)(4-oxo-4H-1,3-benzothiarin-2-yl)methylene]-, dimethyl ester (9CI) (CA INDEX NAME)

78959-06-5 CAPLUS 1,3-Dithlole-4,5-dicarboxylic acid, 2-[(4-chlorophenyl)(4-oxo-4H-1,3-benzothiazin-2-yl)methylene]-, dimethyl ester (9CI) (CA INDEX NAME)

78959-07-6 CAPLUS 1,3-Dithiole-4,5-dicarboxylic acid, 2-[(4-methylphenyl)(4-oxo-4H-1,3-benzothiazin-2-yl)methylene]-, diethyl ester (9CI) (CA INDEX NAME)

ANSWER 28 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

L4 ANSWER 29 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1980:567097 CAPLUS

DOCUMENT NUMBER: ORIGINAL REFERENCE NO.: 93:167097 93:26599a,26602a

TITLE:

93:26599a,26602a
Studies in organic mass spectrometry. I. Electror impact-induced fragmentation of 2-substituted 4H-1,3-benzothiazin-4-ones
Ceraulo, Leopoldo; Agozzino, Pasquale; Ferrugia, Mirella; Giannola, Libero Italo
Fac. Farm., Univ. Palermo, Palermo, I-90123, Italy Annali di Chimica (Rome, Italy) (1977), 67(9-12), 707-19 CORPORATE SOURCE:

North Properties)

(Name of Colombia Co

AUTHOR(S):

L4 ANSWER 30 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1978:509206 CAPLUS
DOCUMENT NUMBER: 89:109206
ORIGINAL REFERENCE NO.: 89:16821a,16824a
TITLE: Heterocycles by reaction of mercapto- and hydroxycarboxylic esters with activated nitriles
AUTHOR(S): Satzinger, Gerhard
CORPORATE SOURCE: Forschungsinst., Goedecke A.-G., Freiburg/Br., Fed. Rep. Ger.
SOURCE: Justus Liebigs Annalen der Chemie (1978), (3),
473-511

CODEN: JLACBF; ISSN: 0075-4617 Journal German CASREACT 89:109206

DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S): GI

The title reaction of RR1CHCN (R = H, Ph; R1 = CO2Et, CN, Bz, Ph,

AB The title reaction or RALDON II. ..., ..., Pyridyl, indolyl, CONH2, etc.) with HSXCO2R2 (X = CH2, CHPh, CEt2, CH2CH2, o-C6H4; R2 = Me, Et), HOCHR3CO2R2 (R3 = H, Ph, p-tolyl, 2-furyl, 2-pyridyl; R2 = Et, Bu), and ENCH2CO2Et gave heterocycles I (R = H, Ph; R1 = CO2Et, CN, Bz, etc.; X = CH2, CHPh, CEt2, o-C6H4, 2-furylmethylene, etc.; XI = O, S, NH), which existed in equilibrium with II. These compds. were alkylated

NB), which existed in equilibrium with II. These compds. were alkylated he ring N in the form of I, usually with the fixation of Z-configuration; under more severe conditions, some were also alkylated at C-3. The ring of I, especially when XI = S, was very stable; thus, I reacted with electrophiles at the 5- or a-position without ring cleavage. I (R = H, RI = CN, X = 0-C6H4, XI = S) and its alkylation products were hydrolyzed to the resp. carboxylic acids or amides, e.g., I (RI = CO2H, CONH2) without disturbing the heterocyclic ring. The alkylation products III (R2 = EtO, BuO, Ph; R3 = Me, MeZNCHZCH2, 2-piperidinoethyl) underwent ring expansion to IV upon prolonged contact with EtJN. Some I and their products are useful as choleretic, diuretic, antimycotic, and central depressive agents (no data).

67433-02-7P 67433-03-8P 67433-04-9P

67433-05-0P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) 67433-02-7 CAPLUS

4H-1,3-Benzothiazine-2-acetonitrile, 4-oxo- (CA INDEX NAME)

L4 ANSWER 30 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

67433-03-8 CAPLUS 4H-1,3-Benzothiazine-2-acetic acid, 4-oxo-, ethyl ester (CA INDEX NAME)

67433-04-9 CAPLUS 4H-1,3-Benzothiazin-4-one, 2-(phenylmethyl)- (CA INDEX NAME)

67433-05-0 CAPLUS 4H-1,3-Benzothiazine-2-acetamide, 4-oxo- (CA INDEX NAME)

Page 25

ANSWER 31 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN SSION NUMBER: 1976:421262 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: ORIGINAL REFERENCE NO.: 85:21262 85:3473a,3476a

TITLE:

AUTHOR(S):

ORPORATE SOURCE: SOURCE:

85:3473a,3476a
Synthesis of 2,2- and 2,4-substituted
1,3-benzthiazines
Szabo, J.; Varga, I.
Dep. Pharm. Chem., Med. Univ., Szeged, Hung.
Acta Chimica Academiae Scientiarum Hungaricae (1976),
88(1), 61-6
CODEN: ACASA2; ISSN: 0001-5407
JOURNAL

DOCUMENT TYPE:

DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S): GI English CASREACT 85:21262

Alkylbenzothiazinones (I, R = H, Rl = Et, PhCH2; R = MeO, Rl = Et, Bu, PhCH2) were obtained in 19.5-38.28 yields by alkylation of the corresponding benzothiazinone with RIMRX (X = halo). Analogously

56755-15-8P

50:03-15-09 (Preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and alkylation of) (preparation and alkylation of) 56:755-15-8 CAPLUS (Preparation and alkylation of) (CA INDEX NAME)

L4 ANSWER 32 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1976:4880 CAPLUS
OCCUMENT NUMBER: 84:4880
CRIGINAL REFERENCE NO.: 84:625a,828a
TITLE: Cyanogen-2-mercaptobenzoic acid condensations. Route to bis-1,3-benzothiazin-4-ones
AUTHOR(S): Heindel, Ned D.; Schaeffer, Lee A.
CORPORATE SOURCE: SOURCE: Journal of Heterocyclic Chemistry (1975), 12(4), 783-4

author(s): CORPORATE SOURCE: SOURCE: 783-4

CODEN: JHTCAD; ISSN: 0022-152X

CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE: JOURNAL
LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB The bisbenzothiazinones I (R = Rl = H, Cl; R = Cl, Me, Rl = H) were

prepared

(21-95%) by treating 2,3,5-(HS)RIRC6H2C02H with NCCN.

IT 57446-11-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 57446-11-4 CAPLUS

CN 4H-1,3-Benzothiazine-2-carboxamide, 6-methyl-4-oxo- (CA INDEX NAME)

L4 ANSWER 31 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

L4 ANSWER 33 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1975:547442 CAPLUS ORIGINAL REFERENCE NO. 83:23163a,23166a TITLE: Reaction of 4H-1,3-benzothiazir

L4 ANSWER 33 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 975:547442 CAPLUS
OCCUMENT NUMBER: 83:127442
ORIGINAL REFERENCE NO: 83:23163a,23166a
Reaction of 4H-1,3-benzothiazin-4-ones with Grignard reagents
AUTHOR(S): Varga, Istvan; Szabo, Janos; Sohar, Pal
CORPORATE SOURCE: Pharm.-Chem. Inst., Med. Univ. Szeged, Szeged, Hung.
COEDENT TYPE: COEDEN: CHEEAN; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASEACT 83:147442
CASEACT 83:147442
CASEACT 83:147442
CASEACT 81:14742
AB Benzothiazinone I reacted with Grignard reagents RIMGBr to give dihydrobenzothiazinone II (R = H, MeG; RI = Ph.) PhCH2MgBr gave, in addition to II (R = MeO, RI = CAPPh), benzylidenebnzthiazine IV, probably addition to II (R = reco, ...
probably
formed via intermediate III (R = MeO, R1 = CH2Ph).

IT 7474-08-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with Grignard reagent)
RN 7474-08-0 CAPLUS
CN 4H-1,3-Benzothiazin-4-one, 2-phenyl- (CA INDEX NAME)

TT

56755-15-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with Grignard reagents)
56755-15-8 CAPLUS
4H-1,3-Benzothiazin-4-one, 6,7-dimethoxy-2-phenyl- (CA INDEX NAME)

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ANSWER 34 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN SSION NUMBER: 1969:491408 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: ORIGINAL REFERENCE NO.: 71:91408 71:17019a,17022a

TITLE:

AUTHOR(S):

71:17019a,17022a Synthesis and study of 1,3-benzothiazines. II. Chemical study of the compounds obtained Bourgoin-Legay, Daniele; Boudet, Roger Lab. Chim. Org., Fac. Sci. Dakar, Dakar, Senegal Bulletin de la Societe Chimique de France (1969), CORPORATE SOURCE: SOURCE:

2524-30 CODEN: BSCFAS: ISSN: 0037-8968

CODEN: BSCFAS; ISSN: 0037-8968

DOCUMENT TYPE: Journal

LANGUAGE: French
OTHER SOURCE(S): CASREACT 71:91408

AB Treatment of 2-alkyl-4H-1,3-benzothiazines (I) with air or H202 results in

preferential oxidation of the S atom, rather than of the 4-CH2 group. Although the corresponding 2-aryl compds. are resistant to air oxidation, careful treatment with RMnO4 in Me2CO solution leads to either S

Although the statement with RNMO4 in Me2CO solution leads to either S oxidation or 4-CH2 oxidation, or to oxidation at both positions, depending on exact conditions. Reaction of I with AgNO3 and alkylation with MeI results in exclusive substitution at the 4-position. A number of other oxidation, substitution, and addition reactions are described. Refluxing 0.7 g. 2-methyl-4H-1,3-benzothiazine (II) in 20 ml. concentrated HCl 24 hrs. and basification gave 0.3 unchanged II, but further treatment of the alkaline filtrate with BrCl yielded 50% N,S-dibenzoyl derivative of 2-mercaptobenzylamine. Heating 2 g. 2-phenyl-4H-1,3-benzothiazine (III) in 20 ml. 50% H2SO4 6 hrs. gave SO2, 0.4 g. PhCO2H, and 0.5 g. benzisothiazole. Upon being exposed to air 2 months., I g. II afforded approx. 0.5 g. 2-methyl-1-oxo-4H-1,3-benzothiazine (IV), m. 158° (EtOH). Similarly prepared were 2-oxthyl-1-oxo-4H-1,3-benzothiazine, m.

137-8° (EtOH), and 2-isopropyl-1-oxo-4H-1,3-benzothiazine, m. 179-80° (H2O-EtOH). Treatment of 1 g. II in 40 ml. AcOH with 40 ml. dilute H2O2 4.5 hrs. afforded 64% IV. Under these conditions, V was obtained in 72% yield, but 2-(p-anisyl)-4H-1,3-benzothiazine (VI)

remained unaffected. A solution of 4.5 g. III in 270 ml. Me2CO was stirred with

10.2 g. KMnO4 4 hrs., kept another 12 hrs., filtered, evaporated, and the residue

extracted with PrOH to give 4-oxo-2-phenyl-1,3-benzothiazine (VII), m. 122.5-3°. Reaction of 1 g. III with 2 g. RMmo4 in 60 ml. Me2CO 3 hrs., addition of 20 ml. concentrated HCl and dilution with 200 ml. H2O afforded 0.3

dea 0.3 g. 2,3-dihydro-1,4-dioxo-2-phenyl-1,3-benzothiazine (vIII), m. 203-4°, and 0.1 g. mixture containing VII and VIII. Stirring a mixture

1 g. 2,3-dihydro-4-oxo-2-phenyl-1,3-benzothiazine and 1 g. KMnO4 in 30

ml. Me2CO at room temperature 24 hrs., heating on a steam bath 1 hr., and

addition of 10 ml. concentrated HCl and 150 ml. H2O yielded 0.3 g. VIII. Starting from VI,

ANSWER 34 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

ANSWER 34 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued) 2-(p-anisyl)-4-oxo-1,3-benzothiazine, m. 178.5-9.5° (PrOH), and 2-(p-anisyl)-2,3-dihydro-1,4-dioxo-1,3-benzothiazine, m. 221° (PhCOZEt), were prepd. via similar procedures. Likewise, oxidn. of 2-(p-bromophenyl)-4H-1,3-benzothiazine (IX) led to 2-(p-bromophenyl)-4H-1,3-benzothiazine (IX) led to 2-(p-bromophenyl)-4-oxo-1,3-benzothiazine, m. 207° (PhCOZEt). Under these conditions, II yielded only tar. A soln. of 1 g. 2-ethyl-4H-1,3-benzothiazine in 10 ml. EtoH was treated with 3 g. AgNO3 in

5 ml. H2O and 20 ml. EtoH, the insol. Ag salt salt added to a soln. of 1 ml. MeI in 30 ml. PhMe, and the mixt. stirred at room temp. 1 hr. and at 50° 2.5 hrs. to give 0.64 g. 2-ethyl-4-methyl-1,3-benzothiazine, m. 80-1° (C6He-petr. ether). Similar reaction of IV furnished an unstable Ag salt which was treated directly with MeI in EtoH at room

to give 2,4-dimethyl-1-oxo-1,3-benzothiazine, m. 102° (CC14).

Dropwise addn. of 6 ml. 20% Br in CC14 to 1 g. III in 30 ml. CHC13 gave 1.3 g. red solid, C14HilBr2NS, m. 145°. Treatment of this compd. with hot PrOH gave VII. Brominations were likewise studied with VI, IX, and 2-(p-nitrophenyl)-4H-1,3-benzothiazine, but complex mixts. of

and 2-(p-...
products
were obtained.
IT 7474-08-0P 23574-20-1P 23574-21-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 7474-08-0 CAPLUS
CN 4H-1,3-Benzothiazin-4-one, 2-phenyl- (CA INDEX NAME)

23574-20-1 CAPLUS
4H-1,3-Benzothiazin-4-one, 2-(p-methoxyphenyl)- (8CI) (CA INDEX NAME)

23574-21-2 CAPLUS 4H-1,3-Benzothiazin-4-one, 2-(p-bromophenyl)- (8CI) (CA INDEX NAME)

ACCESSION NUMBER: DOCUMENT NUMBER:

ORIGINAL REFERENCE NO.:

ANSWER 35 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN
SSION NUMBER: 1967:443770 CAPLUS
MENT NUMBER: 67:43770
INAL REFERENCE NO: 67:8227a,8230a
E: Lithium aluminum hydride hydrogenation test on a
1,3-benzothiazine
OR(S): Bourgoin-Legay, Daniele; Boudet, Roger
Univ. Dakar, Dakar, French West Africa
CC: Univ. Dakar, Dakar, French West Africa
CC: CC: Comptes Rendus des Seances de l'Academie des AUTHOR (S)

AUTHOR(S):
CORPORATE SOURCE:
SOURCE:
Sciences,

Sciences,

Serie C: Sciences Chimiques (1967), 264(15), 1304-6
CODEN: CHDCAQ; ISSN: 0567-6541
JOURNAL JOURNAL
LANGUAGE: French
GI For diagram(s), see printed CA Issue.
AB The reduction of 2-phenyl-4-oxo-1,3-benzothiazine (I) with LiAlH4 led,
unexpectedly, to 3 products: 2-mercaptobenzylamine (Ia), benzisothiazole
(II), and benzyl alc. These provided an interesting confirmation of the
initial structure. I (9.6 g.) was treated with 2.5 g. liAlH4 in 50 ml.
anhydrous ether. The mixture was extracted 6 hrs., heated 5 hrs.,
cooled, 10 ml.

cooled, 10 ml.

EtOAc added carefully, and then 70 ml. 1:1 HCl-H2O added. The aqueous

was made alkaline, and approx. 1 g. benzisothiazole was obtained.

Excess BzCl (15 ml.) was added to the aqueous solution to yield 10 g. precipitate, m. 141°, identical with the N,S-dibenzoylated derivative of Ia (CA 64: 15782e).

identical with the N,0-virenegaline
Evaporation
of the solvent from the ether phase and distillation of the residue
yielded 3.8
g. benzyl alc.
IT 7474-08-0
DOM (Paragraph): RACT (Reactant or reagent)

RE: RCT (Reactant); RRC1 (Reactant or reagent) (reduction of, with lithium tetrahydroaluminate) 7474-08-0 CAPLUS 4H-1,3-Benzothiazin-4-one, 2-phenyl- (CA INDEX NAME)

L4 ANSWER 36 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1962:475956 CAPLUS DOCUMENT NUMBER: ORIGINAL REFERENCE NO.: 57:75956 57:15105c-q 57:15105c-q Synthesis and biological activity of some 4-(substituted-amino)pyrimidines Segal, Hayim; Hedgooth, Charles; Skinner, Charles G. Univ. of Texas, Austin Journal of Medicinal & Pharmaceutical Chemistry (1962), 5, 871-6 CODEN: JMPCAS; ISSN: 0095-9065 TITLE: AUTHOR(S): ORPORATE SOURCE: SOURCE: DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB A series of 13 4-(substituted-amino)pyrimidines were prepared and tested DOCUMENT TYPE: their effect on the rate of seed germination. None of the compds. nce
the rate of germination and all were relatively non-toxic to the seed.
From these results as well as earlier tests it appears that the purine
nucleus is essential for producing analogs with kinetin-like activity. A
mixture of 2.88 g. 2,4-dimercaptopyrimidine and 4.88 g. BuMH2 was mixture of 2.88 g. 2,4-dimercaptopyrimidine and 4.00 g. Daniel refluxed 5 hrs., cooled, 50 ml. H2O added, and the precipitate re-crystallized from MeOH to give 3.2 g. 4-butylamino-2-pyrimi-dinethiol, m. 212-14° (decomposition). Prepared similarly were: 4-isopentylamino-2-pyrimidinethiol, m. 198-9° (decomposition); 4-n-hexylamino-2-pyrimidinethiol, m. 200-4° (decomposition); and 4-n-heptylamino-2-pyrimidinethiol, m. 179-80° (decomposition). 4-n-Pentylamino-2-pyrimidinethiol (5.9 g.), 2.83 g. chloroacetic acid, and 35 ml. H2O was heated 1 hr., cooled, evaporated to dryness in vacuo, and the residue recrystd. from MeOH-Me2CO-dioxane to give 4 g. 2-carboxymethylthio-4-n-pentylaminopyrimidine-HCl, m. 143-5° (decomposition). 2-Carboxymethylthio-4-n-pentylaminopyrimidine-HCl (1.28 g.) and 20 ml. concentrated HCl was refluxed 4 hrs., cooled, the pH adjusted to 7 with NH4OH, and the precipitate recrystd. from H2O to give].

4-n-pentylamino-2-pyrimidinol, m. 105-7° (decomposition).

4-n-Hexylamino-2-pyrimidinethiol (3.17 g.), 1.59 g. Na2CO2, and 12 g.

Raney Ni in 100 ml. EtOH was refluxed 24 hrs., filtered while hot, 12 g.

Raney Ni added, refluxed 8 hrs., filtered, the filtrate evaporated to drvness in vacuo, and the residue crystallized from hexane-C6H6 to give 0.8 g.

4-n-hexylaminopyrimidine, m. 61-3°. Prepared similarly were:

4-n-heptylaminopyrimidine-HCl, m. 147-52° (decomposition);

4-benzylaminopyrimidine-HCl, m. 155-7°.

97554-98-98-9, H-1, 3-Benzothiazin-4(3H)-one, 1-ethyl-2-phenyl98681-46-0P, HH-1,3-Benzothiazin-4(3H)-one, 2-phenyl-1-propyl
RL: PREP (Preparation)

(preparation of)
97554-98-8 CAPLUS

1H-1,3-Benzothiazin-4(3H)-one, 1-ethyl-2-phenyl(7CI) (CA INDEX NAME)

L4 ANSWER 36 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

98681-46-0 CAPLUS 1H-1,3-Benzothiazin-4(3H)-one, 2-phenyl-1-propyl- (7CI) (CA INDEX NAME)

L4 ANSWER 37 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1962:475955 CAPLUS
DOCUMENT NUMBER: 57:75955

CRIGINAL REFERENCE NO: 57:15105a-c
Unexpected reaction of alkyl halides with silver derivative of a benzometathiazone
AUTHOR(S): Boudet, Roger
CORPORATE SOURCE: Univ. Dakar, W. Africa
SOURCE: Compt. Rend. (1962), 255, 533-5
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB In 2.4 g. 2-phenyl4,5-benzothiazinone and 80 ml. boiling EtOH was dissolved 2 g. AgNO3 and the mixture cooled to precipitate 3.5 g. I, pale yellow, pale yellow, decomposed at 80°. I, 2 g. MeI, and 50 ml. PhMe stirred 2 hrs. at 50°, the mixture filtered, the filtrate evaporated, and the residue crystallized from EtOH gave 1.5-2 g. 1-methyl derivative (II) of I, m. Hydrolysis of II in boiling H2O gave PhCHO and 2-MeSC6H4CONH2 (III).

Homologs of II made were 1-Et, m. 55°, and 1-Pr, m. 50°.

Corresponding homologs of III were 2-EtS, m. 131-2°, and 2-Prs, m. 123.5°, which was further hydrolyzed to 2-PrSC6H4CO2H, m. 121.5-2.5°.

97283-55-1P, 1H-1,3-Benzothiazin-4(3H)-one, 1-methyl-2-phenyl-97554-98-8P, 1H-1,3-Benzothiazin-4(3H)-one, 1-methyl-2-phenyl-98681-46-0P, 1H-1,3-Benzothiazin-4(3H)-one, 2-phenyl-1-propyl-RL-PRFP (Preparation) RL: PREP (Preparation) (preparation of)
97283-55-1 CAPUUS
18-1,3-8-Bozothiazin-4(3H)-one, 1-methyl-2-phenyl- (7CI) (CA INDEX NAME)

97554-98-8 CAPLUS 1H-1,3-Benzothiazin-4(3H)-one, 1-ethyl-2-phenyl- (7CI) (CA INDEX NAME)

98681-46-0 CAPLUS 1H-1,3-Benzothiazin-4(3H)-one, 2-phenyl-1-propyl- (7CI) (CA INDEX NAME)

L4 ANSWER 37 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

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ANSWER 38 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN SSION NUMBER: 1961:27911 CAPLUS ACCESSION NUMBER: DOCUMENT NUMBER: 55:27911 55:5509b-i.5510a-d ORIGINAL REFERENCE NO.: 55:5509b-i,5510a-d Arylbenzo[e]-l,3-thiazine derivatives. III. Verification of the position of the alkoxy groups in arylbenzo[e]-l:3-thiazine derivatives by synthesis Szabo, J.; Vinkler, E. Med. Univ., Szeged, Hung. Acta Chimica Academiae Scientiarum Hungaricae (1958), 17, 201-9 CODEN: ACASA2; ISSN: 0001-5407 TITLE: CORPORATE SOURCE: SOURCE . 17, 201-9
CODEN: ACASA2; ISSN: 0001-5407
DOCUMENT TYPE: Journal
LANGUAGE: German
AB cf. CA 52, 6358c. The position of alkoxy groups in several
dialkoxybenzo[e]-1,3-thiazine derivs. was verified by oxidation of the
benzothiazine bases to 4-oxo derivs., and comparison of these with the
same products obtained from S-aroylthiosalicylamides, the alkoxy
positions
of which were known. The S-aroylthiosalicylamide derivs., which were
prepared from 6,7-dialkoxy derivs. obtained from 6,3,4-HzN(Meo)2C6HZCOZH,
were cyclized to 4-oxo derivs. according to Bohme and Schmidt (cf. CA 49.
15907a). Thus, 2.85 g. 2-phenyl-6,7-dimethoxybenzo[e]-1,3-thiazine in 10
ml. HOAc treated with 1.35 g. Cro3 in 1ml. H2O and 2 ml. HOAc gave after
10 min. 0.8 g. 2-phenyl-4-oxo-6,7-dimethoxybenzo[e]-1,3-thiazine (I),
yellow needles, m. 183-90 (alc.). Similarly prepared were from
0.86 g. 2-(3,4-dimethoxyphenyl)-4-oxo-6,7-dimethoxybenzo[e]-1,3-thiazine, 0.25
g. 2-(3,4-dimethoxyphenyl)-4-oxo-6,7-dimethoxybenzo[e]-1,3-thiazine (II),
yellow needles, m. 217-18° (alc.). from 1.73 g.
2-phenyl-6,7-diethoxybenzo[e]-1,3-thiazine (III),
yellow needles, m. 217-18° (alc.). from 1.73 g.
2-phenyl-6,7-diethoxybenzo[e]-1,3-thiazine (III),
yellow needles, m. 217-18° (alc.). from 1.73 g.
2-phenyl-6,7-diethoxybenzo[e]-1,3-thiazine (III),
yellow needles, m. 217-18° (alc.). from 1.73 g.
2-phenyl-6,7-diethoxybenzo[e]-1,3-thiazine (III),
yellow needles, m. 217-18° (alc.). from 1.73 g.
2-phenyl-6,7-diethoxybenzo[e]-1,3-thiazine (III),
yellow needles, m. 217-18° (alc.). from 1.73 g. (alc.). concentrated

HCl added at 0° to 3.45 g. NaNO2 in 15 ml. H2O, the mixture stirred 1 ht. at 07, added with stirring to a solution prepared from 13 G. Na2S, 15 ml. H2O, and 1.73 g. S, treated with 2.11 g. NaOH in 100 ml. H2O and with 50 g. crushed ice, the mixture stirred 3 hrs. until N evolution

ceased, acidified with HCl, the precipitate filtered off, washed with H2O, dissolved in

dissolved in

dilute NaHCO3, treated with C, precipitated with concentrated HCl,
filtered, washed with

H2O, suspended in 50 ml. HOAc, 2 g. Zn added, the mixture refluxed 3

cooled, centrifuged, the precipitate heated 15 min. with 10 g. NaOH in 50 ml

H2O, filtered, the solution acidified with HCl, and the precipitate filtered off,

red off, washed with H2O, and dried gave 4.6 g. 4,5-dimethoxythiosalicylic acid (IV), needles, m. 184-5° (alc.). IV (4.3 g.) in 25 ml. alc. treated with a saturated alc. iodine solution until just colored brown,

added, the precipitate formed filtered off, washed with 50% alc., and lat 105° gave 3.95 g. 4,4',5,5'-tetramethoxydiphenyl

ANSWER 38 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued) disulfide-2,2'-dicarboxylic acid (V), needles, m. 248-50° (alc.). V (8.52 g.) dissolved on the H2O bath in a soln. of 4 g. KHCO3 in 30 ml. H2O, evapd. to dryness at 105°, the residue pulverized, suspended in 50 ml. C6H6, gradually treated with 10 g. SOC12, refluxed 30 min., the solvent and SOC12 distd. in vacuo, the mixt. cooled, and the crystals formed washed with 15-20 ml. petr. ether gave 7.2 g. 4,4',5,5'-tetramethoxydiphenyl disulfide-2,2'-dicarboxnlc children (VI), yellow needles, m. 147-8° (C6H6). VI (6.95 g.) treated in 60 ml. C6H6 satd. with dry NH3, gave 5.2 g. 4,4',5,5'-tetramethoxydiphenyl disulfide-2,2'-dicarboxamide (VII), needles, m. 221-3° (alc.). VII (4.24 g.) in 20 ml. HOAc treated with 1 g. Zn powder, and the mixt. refluxed 1 hr. gave 2.55 g. 4,5-dimethoxythiosalicylamide (VIII), yellow needles, m. 169-70° (alc.). VIII (2.13 g.) in 8 ml. abs. C5H5N gradually treated with 1.4 g. EC1, stirred 30 min., poured into dil. H2SO4 and crushed ice, the product filtered off, washed with H2O, and dried gave 2.3 g. S-benzoyl-4,5-dimethoxythiosalicylamide (TN), needles, m. 179-80° (alc.). Two-thirds of a soln. of 1.59 g. TX in 20 ml. abs. xylene distd. with slow introduction of dry HCl, the remainder of solvent distd. with slow introduction of dry HCl, the remainder of

solvent distd. in vacuo after shutting off the HCl, the residue dissolved in C6H6, washed with N NaOH and H2O, dried, the solvent distd., and the residue crystd. from alc. gave 0.8 g. I, m. 189-90°. VIII (1.07 g.) treated with 3,4 (MeO)2C6H3COCl as in the prepn. of IX gave 1.3 g. S-veratroyl-4,5-dimethoxythiosalicylamide (X), needles, m. 178-9° (alc.). X (0.35 g.) treated as in the prepn. of I gave 0.4 g. II, m. 217-18° (alc.). oc6H4(CEL)2 (41.5 g.) and 45 g. PNNMCHO in 51 g. POCl3 refluxed 90 min. on a H2O bath, the mixt. poured into 50 ml.

217-18° (alc.). O-C-84 (DEC) (41.5 g.) and 45 g. PRINGELO IN 51

H2O, POCCIS refluxed 90 min. on a H2O bath, the mixt. poured into 50 ml.

H2O, extd. with 200 ml. Et2O, washed with H2O, shaken 3 hrs. with 40 g. NaHSO3 in 120 ml. H2O, the aq. phase sepd., treated with solid Na2CO3, the freed aldehyde extd. with Et2O, the Et2O layer washed with H2O, dried, the solvent distd., and the residue distd. in vacuo gave 26.6 g. 3,4-(KDO)2CGH3CHO (XII), wellow ne2LsO, n21.50 l.557, d21.5 l.101. XI (38.8 g.) nitrated with 60.5 g. conod. HNO3 gave 43 g. 6,3,4-2N(Et0)2CGH2CHO (XII), yellow needles, m. 95-6° (alc.). XII (23.9 g.) and 12 g. NaOH in 200 ml. H2O warmed on the H2O bath, gradually treated with 80 g. RMnO4 in 600 ml. H2O warmed on the H2O bath, gradually treated with 80 g. RMnO4 in 600 ml. H2O warmed on the H2O bath, gradually treated with 10.5 g. hin 250 ml. alc. hydrogenated at 50° and atm. pressure with 0.05 g. Pd-C gave 10.1 g. 6,3,4-R2N(EHO)2CGH2COH (XIV), prisms, m. 135-6° (decompn.) (alc.). XIV (9 g.) treated as in the prepn. of IV gave 4 g. 4,5-diethoxythiosalicylic acid (XV), needles, m. 202-3° (alc.). XW (3.63 g.) treated as in the prepn. of VI gave 7.4 g. 4,4',5,5'-tetraethoxydiphenyl disulfide-2,2'-dicarboxylic acid (XVI), prisms, m. 239-40° (alc.). XVI (9.25 g.) treated as in the prepn. of VI gave 7.4 g. 4,4',5,5'-tetraethoxydiphenyl disulfide-2,2'-dicarboxylic acid (XVII), yellow needles, m. 106-9° (C6H6 and petr. ether). XVII (5.19 g.) treated as in the prepn. of VII gave 7.4 g. 4,4',5,5'-tetraethoxydiphenyl disulfide-2,2'-dicarboxylic acid (XVII), yellow needles, m. 106-9° (C6H6 and petr. ether). XVII (5.19 g.) treated as in the prepn. of VII gave 4 g. 4,4',5,5'-tetraethoxydiphenyl disulfide-2,2'-dicarboxylic acid (XVII), yellow needles, m. 110-19° (C6H6 and petr. ether). XVII (5.19 g.) treated as in the prepn. of VII gave 4 g. 4,4',5,5'-tetraethoxydiphenyl disulfide-2,2'-dicarboxylic acid (XVII), predeles, m. 219-20° (C6H6 and petr. ether). XVII (5.19 g.) treated as in the prepn. of VII gave 4 g. 4

ANSWER 38 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued) the prepn. of IX gave 2.14 g. S-benzoyl-4,5-diethoxythiosalicylamide

the prepn. of 1X gave 2.14 g. S-benzoyl-4,5-daethoxythiosalicylamid, needles, m. 179-80° (alc.). XX (1.73 g.) treated as in the prepn. of I gave 0.9 g. III, m. 154-5° (alc.). 56755-15-8P, 4H-1,3-Benzothiazin-4-one, 6,7-dimethoxy-2-phenyl-101734-2-3P, 4H-1,3-Benzothiazin-4-one, 6,7-diethoxy-2-phenyl-101734-79-6P, 4H-1,3-Benzothiazin-4-one, 2-(3,4-dimethoxy-phenyl)-6,7-dimethoxyRI: PREP (Preparation) (preparation of) 56755-15-8 CAPLUS 4H-1,3-Benzothiazin-4-one, 6,7-dimethoxy-2-phenyl- (CA INDEX NAME)

101734-42-3 CAPLUS 4H-1,3-Benzothiazin-4-one, 6,7-diethoxy-2-phenyl- (CA INDEX NAME)

101734-79-6 CAPLUS 4H-1, 3-Benzothiazin-4-one, 2-(3,4-dimethoxyphenyl)-6,7-dimethoxy- (CA INDEX NAME)

ANSWER 39 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1960:118326 1960:118326 CAPLUS
54:12826
54:22656h-i,22657a-b
Studies on thiazine: oxobenzo-m-thiazine and some of
its 2-(alkylaminomethyl) derivatives
Conti, L.; Spinelli, D.
Univ. Bari, Italy
Bollettino Scientifico della Facolta di Chimica
Industriale di Bologna (1959), 18, 29-33
CODEN: BSPCAY; ISSN: 0366-3205
Journal
Unavailable ORIGINAL REFERENCE NO.: AUTHOR (S) CORPORATE SOURCE: SOURCE: COEN: BSFCAY; ISSN: 0366-3205
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. Conti and Leandri, CA 51, 5765; 51, 17926a; 51, 17927g. New
thiazine
derivs. of potential pharmacol. interest were prepared in view of earlier
and related work. 4-Oxobenzo-m-thiazine-2-carboxylic acid (I), m.
107° (BtOH), was prepared by adding 3.3 g. freshly distilled Etc2CCN to
4.5 g. thiosalicylic acid in 20 ml. anhydrous dioxane, cooling the ice and salt, passing in a stream of dry HCl 3 hrs., allowing the

mixture to stand overnight at 0°, filtering, neutralizing the aqueous suspension of the precipitate with NaHCO3 over ice, and working up the solid precipitate (6 g. crude). 4-Cxobenzo-m-thiazine (II), C8H5NOS, sweetish taste, m. 138° (H2O), was prepared by boiling 1 g. I in 100 ml. H2O to solution and taking to near dryness. Et ester of 4-cxobenzo-m-thiazine-2-acetic acid, needles, m. 172° (RtOH and dioxane), was prepared analogously from 3 g. thiosalicylic acid and 2.4 g. EtO2CCH2CN in 20 ml. dioxane in 2.5-g. yield. 2-Chloromethyl-4-oxobenzo-m-thiazine, (III), m. 115° (benzene and a little absolute alc.), was similarly prepared in 3.1-g. yield

vield t from 3.3 g. thiosalicylic acid and 1.62 g. CICHZCN in 25 ml. anhydrous dioxane; it was not stable in air. 2-Morpholinomethyl derivative of II,

157° (C6H6), 2-piperidinomethyl derivative of II, needles, m. 149° (C6H6), 2-diethylaminomethyl derivative of II, platelets, m. 160° (alc.-C6H6), and 2-cyclohexylaminomethyl derivative of II, needles, m. 185° (C6H6 and petr. ether), were prepared by refluxing mole III and 2.5 moles of the resp. amine in C6H6 and working up the

products.
67433-03-09, 4H-1,3-Benzothiazine-2-acetic acid, 4-oxo-, ethyl ester 95591-85-6P, 4H-1,3-Benzothiazine-2-carboxylic acid, 4-oxo- 98592-32-6P, 4H-1,3-Benzothiazine-4-one, 2-(chloromethyl)-100115-33-6P, 4H-1,3-Benzothiazin-4-one, 2-(diethylaminomethyl)-100795-37-7P, 4H-1,3-Benzothiazin-4-one, 2-morpholinomethyl-101938-35-6P, 4H-1,3-Benzothiazin-4-one, 2-(cyclohexylaminomethyl-101938-35-6P, 4H-1,3-Benzothiazin-4-one, 2-piperidinomethyl-Ri-PKEP (Preparation)
(preparation of)
67433-03-38 CAPLUS
4H-1,3-Benzothiazine-2-acetic acid, 4-oxo-, ethyl ester (CA INDEX NAME)

L4 ANSWER 39 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

98591_85_6 CAPLIES

4H-1,3-Benzothiazine-2-carboxylic acid, 4-oxo- (CA INDEX NAME)

98592-32-6 CAPLUS 4H-1,3-Benzothiazin-4-one, 2-(chloromethyl)- (CA INDEX NAME)

100615-33-6 CAPLUS 4H-1,3-Benzothiazin-4-one, 2-(diethylaminomethyl)- (6CI) (CA INDEX NAME)

100795-37-7 CAPLUS 4H-1,3-Benzothiazin-4-one, 2-morpholinomethyl- (6CI) (CA INDEX NAME)

L4 ANSWER 39 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

100957-60-6 CAPLUS

4H-1,3-Benzothiazin-4-one, 2-(cyclohexylaminomethyl)- (6CI) (CA INDEX NAME)

101938-35-6 CAPLUS 4H-1,3-Benzothiazin-4-one, 2-piperidinomethyl- (6CI) (CA INDEX NAME)

L4 ANSWER 40 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1960:97610 CAPLUS
DOCUMENT NUMBER: 54:97610
CRIGINAL REFERENCE NO.: 54:18530E-i,18531a-b
Sulfuration of organic compounds. XIX. Synthesis of
3,1-benzothiazine-4-thiones and corresponding
oxygenated compounds
Legrand, Louis
COMPORATE SOURCE: Fac. sci., Caem
Bulletin de la Societe Chimique de France (1960)
337-43
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. CA 54, 13103b. o-RCONNEC6H4CO2R' (I) (from RCOCl and o-H2CC6H4CO2R',
except when R' = H) (20 g.), refluxed 1 hr. with 40 g. P255 in 500 cc.
xylene, the solution cooled, brought to 1 l. with C6H6, filtered, the
filtrate washed with cold 5% KOH and with H2O, H9Cl2 in Me2CO added, the
addition compound filtered, washed with Et2O, and decomposed with
aqueous Na2S, or,
if the addition compound is soluble, the solvent evaporated, gives
2-R-3,1-benzothiazin-4-thione (II), red or orange crystals. To 1 g. II
in 150 cc. boiling Me2CO is added powdered RMnO4 to give a quant. yield
of

2-R-3,1-benzothiazin-4-one (III) [when R = aryl, 1 g. II in 50 cc. ling AcOH is oxidized to 90-5% III by 2 g. Hg(OAc)2]. R, R', m.p. of I, yield of II, m.p. of II, and m.p. of III are: H, H, 168°, 5, 114°, 122°, Me, H, 188°, 6 (Me, Me 80%), 99°, 93°, Et. Me, 34° (bl 140°), 15, 63°, -; iso-Pr, Me, 49-5;° (bl 136°), 19, 91°, -; tert-Bu, Me, 46-7° (bl 128-30°), 80, 80°, -; PhCH2, Me, 45° (bl 200-3°), 30, 148°, 90°; Ph, H, 181°, 8 (Ph, Me 35%; Ph, Et 33%), 128°, 116°; 2-MecGH4, Me, 38°, 32, 116°, Et, 103°; 4-MecGH4, Me, 114°, 37, 144°, 173°; 2-ClcGH4, Et, 115°, 43, 145°, 137, 144°, 173°; 2-ClcGH4, Et, 115°, 43, 145°, 138°, 44-ClcGH4, Me, 186°, 32, 197°, 123°; 4-BcCGH4, Et, 23°, 34, 211°, 199°; 2-O2NCGH4, Me, 156°, 50, 147°, 189°, 3-O2NCGH4, Et, 127°, 29, 184°, 166.5°; 1-ClOH7; Me, 120°, 50, 171.5°, 156°; 2-ClOH7, 129°, 50, 157.5°, 157°. Similarly, 2,5-(KCOMH)ClcGH3CoZMe (IV) gives 2-R-6-chloro-3,1-benzothiazine-4-thione (V) and 2-R-6-chloro-3,1-benzothiazine-4-doe (V) and 2-R-6-chloro-3,1-benzothiazi 2-R-3,1-benzothiazin-4-one (III) [when R = aryl, 1 g. II in 50 cc.

solution is concentrated and AcOH added to give crystals of unstable o-RCONHCGH4COSH, which, heated at 120-60°, gives approx. 80% (from II) 2-R-3,1-benzoxazin-4-one (VII). R and m.p. of VII are: Ph, 123°; 2-McG6H4, 116°; 4-McG6H4, 156°; 2-C1C6H4, 136°; 4-C1C6H4, 189°; 2-BrC5H4, 120.5°; 3-BrC5H4, 159°; 2-C10H7, 206.5°. Similarly, V gives the following 2-R-6-chloro-3,1-benzoxazin-4-ones (R and m.p. shown): Ph, 196°;

2/13/2008 Habte

ANSWER 40 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued) 4-ClC6H4, 194°. II (R = Ph) (VIII) with H2O2 and K in alc.-H2O gives o-PhCONHC6H4CO2H. VIII is formed from III (R = Ph) or VII (R = Ph) heated with P2S5 in xylene. 98592-33-7 (Derived from data in the 6th Collective Formula Index (1957-1961)) 98592-33-7 CAPLUS

4H-1,3-Benzothiazin-4-one, 6-chloro-2-methyl- (CA INDEX NAME)

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ANSWER 41 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN SSION NUMBER: 1960:97609 CAPLUS ACCESSION NUMBER: DOCUMENT NUMBER: ORIGINAL REFERENCE NO.: 54:97609 54:18529g-i,18530a-f 54:18529g-1,189.3Ua-T Chlorination and bromination of cyclic acetals Cort, L. A.; Pearson, Ronald G. Battersea Coll. Technol., London Journal of the Chemical Society (1960) 1682-7 CODEN: JCSOA9; ISSN: 0368-1769 TITLE: CORPORATE SOURCE: SOURCE: DOCUMENT TYPE. Journal Unavailable LANGGAGE: Unavailable
COTHER SOURCE(S): CASREACT 54:97609
AB Cl was fed into 55 g. molten trans-1,4,5,8-tetraoxadecahydronaphthalene
(I), prepared according to Contardi and Ercoli (CA 31, 17644 in the ence of a crystal of iodine at 140° until 1 mole was absorbed. Distillation gave 4.2 g. fraction, b0.6 134-52°, from which was obtained 2,3-dioxo-1,4-dioxane, m. 144-5.5°, infrared absorption (broad band) 170 cm.-1. During chlorination, 60 g. volatile material was passed
through a H2O-condenser and trap at 0° to give 1.4 g. liquid condensate; no solid derivative could be obtained with KOH and α-naphthol in EtOH from the liquid fraction (0.35 g.). b764
80-98°. I (67 g.) chlorinated as above, continued until 0.5 mole was absorbed, and the mixture held 5 hrs. at 80-95°/17 mm. gave 22.6 g. sublimate, m. 133-8° (CC14) and a liquid residue, which, on distillation, gave 11.3 g. distillate, b0.2 98-150° and 14.5 g. residue which did not distil at 245°/0.2 mm. Di-2-bromoethyl oxalate (Ia), m. 55.0-5.5° (C6H6-ligroine) was obtained from H2C204 (64% yield) by the method of Contardi, et al. I (19.5 g.) and 25.2 g.
N-bromosuccinimide (II) was heated in a sealed tube 22 hrs. at 120°, the product extracted with CC14, the CC14 distilled, and the residue 120°, the product extracted with con., residue

(4.2 g.) held 4 hrs. at 85°/14 mm. ((0.22 g.) unchanged I sublimed) to give 0.5 g. unsublimed Ia, m. 55.0-5.5 (C6H6-ligroine), infrared absorption 4000-650 cm.-1, strong at 1774 and 1745. 1,3-Dioxolane (III) (266 g.) containing 0.5 g. lodine was chlorinated at the b.p. (exothermic reaction) to constant weight (3 days), the product distilled at atmospheric pressure, and the main fraction distilled 3 more times to give 185 g. 2-chloroethyl formate ate (IIIa), b763 131-2°, n25D 1.4251. Br (294 g.) was added dropwise to 136 g. III at 0° to give 425.5 g. product which, on repeated distillation in vacuo, gave 37 g. 2-bromoethyl formate (IV), b765 147-9°, b13 44.0-0.5, n25D 1.4611; approx. the same yield of IV was obtained with all distns. except the 1st at atmospheric pressure. Evidence is given rearrangement of α -chloroacetals comparable with that for α -bromoacetals. Bromination of 23.5 g. III in 25 ml. CCl4 with 50 g. II and distillation in vacuo gave 13.4 g. IV, b13 44.0-4.5, n25D 1.4611, a fraction, b13 124-5°, after hydrolysis with H2O at 80° and treatment with Brady's reagent, gave, as derivs. (separated with EtOH),

ANSWER 42 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN SSION NUMBER: 1960:56490 CAPLUS ACCESSION NUMBER: 1960:156490 CAPLUS
DOCUMENT NUMBER: 54:56490
CRIGINAL REFERENCE NO.: 54:1033f-h
TITLE: A new heterocyclic system of the benzo[4,5]m-thiazine type. II
AUTHOR (S): Boudet, Roger
CORPORATE SOURCE: Fac. Scis., Dakar
SOURCE: Bulletin de la Societe Chimique de France (1959)
1791-3
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB ef. C.A. 49, 5376e. By condensation of PhCCl3 with 2-mercaptobenzamide
(I) in the presence of Zn in p-xylene, 2-phenylbenzo[4,5]-m-thiazin-6-one
(II) was obtained. II was chemical inert against the usual reagents, except ACCESSION NUMBER: AUTHOR (S) except

H2SO4. This great stability is apparently due to considerable resonance stabilization. A suspension of 20 g. Zn derivative of II in 16.5 ml. PhCCl3 and 200 ml. anhydrous p-xylene was slowly heated under vigorous stirring 6--8 hrs. until the HCl evolution ceased. After chilling the solvent was distd and the residue dissolved in 100 ml. boiling PrOH. On cooling, 12 g. crude II was isolated and recrystd. from CHCl3 or PrOH to yield 45% m. 108.3-9.0°. II (1 g.) in 20 ml. pure H2SO4 was heated slowly to 40°, until the evolution of SO2 ceased, and, after 24 hrs. at room temperature, ice was added to yield 0.6 g. (o-H2NCOC6H4S)2, m. 249°, and temperature, ice was added to yield 0.0 g. (0-Hz) 0.5 g. Bz0, 4H-1,3-Benzothiazin-4-one, 2-phenyl-Ri: PREP (Preparation) (preparation of) 7474-08-0 CAPLUS IT 4H-1,3-Benzothiazin-4-one, 2-phenyl- (CA INDEX NAME)

following 2,4-dinitrophenylhydrazones: glyoxal bis-, m. 333-6°

L4 ANSWER 41 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued) (decompn.), and HCHO, m. 164-6° in approx. equal quantities.

Di-2-chloroethyl oxalate (from 2.2 g. H2c2O4) and 2.5 g. p-anizidine (V), heated at 100° and resolidified after 15 min., gave the di-p-anizidide of H2c2O4, m. 263.5-4.5° (C2H2C14 and dioxane-H2C). IIIa (10 g. from III) boiled in 30 ml. C6H6 with 11.3 g. V 1 hr. and the C6H6 removed gave 5.2 g. p-anizidide of H2cO2H, m. 78° (ECOH).
2-Bromoethyl formate (30 g. from III) and 24.1 g. V, heated 1.5 hrs. on a steam bath, the cold mixt. triturated with 10 ml. McOH and after 3 days, the crystals (11.2 g.) collected, gave needles, m. 287-9° (decompn.) (McOH-dioxane); this (3.5 g.) treated with dil. aq. NaOH and Ac2O gave aceto-p-anizidide, m. 127° (H2C)). S-2-2

Hydroxyethylthluronium picrate (VI), m. 234-42° (decompn.), prepd. in the usual way from BrCHCHCOH in EtOH with previous melting at 162-4° and resolidification at 168°, was recovered quant.

after boiling 8 hrs. in Me2CO. IIIa (3.6 g. from III), 5.0 g. NaI, and 3.5 g. (H2N)2CIS was boiled 8 hrs. in 15 ml. Me2CO, 10 g. picric acid added to the cold mixt., then 15 ml. H2O, the mixt. boiled to give a clear soln., evapd. to half vol., and an equal vol. H2O added to give, on cooling, 3.2 g. VI, m. 236-46° (decompn.) (H2O). Repetition of the expt. with 14.5 g. IIIa in Me2CO as solvent at all stages gave 21.1 g.

m. 240-4° (decompn.) (Me2CO-C6H6). Treatment of 3.6 g. IV with (H2N)2 C:S in EtOH gave 3.5 g. VI, m. 242-52° (decompn.) with previous melting and solidification at 163-6°. 98592-33-7 (Derived from data in the 6th Collective Formula Index (1957-1961)) 98592-33-7 CAPLUS 4H-1,3-Benzothiazin-4-one, 6-chloro-2-methyl- (CA INDEX NAME)

L4 ANSWER 43 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1957:99143 CAPLUS
DOCUMENT NUMBER: 51:99143
NRIGINAL REFERENCE NO: 51:17927g-h
AUTHOR(S): Conti, L.; Leandri, G.
CORPORATE SOURCE: Uhiv. Belogna, 17957), 15, 37-9
CORPORATE SOURCE: Bollettino Scientifico della Facolta di Chimica Industriale di Belogna (1957), 15, 37-9
COEN: BSFCAY; ISSN: 0366-3205
DOCUMENT TYPE: Unavailable
AB A new synthesis is described for the preparation of
2-aryl-4-oxo-5,6-benzo-1,3
thiazines, obtained by condensation of thiosalicylic acid with aromatic nitriles in presence of aqueous HCl. Numerous derivs. are described with regard to their possible therapeutic activity. Compds. prepared are
(aryl ANSWER 43 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN regard to their possible therapeutic activity. Compds. prepared are 1 given): Ph, needles, m. 125° (from EtOH); p-O2NC6H4, yellow prisms, m. 230° (from EtOH-dioxane) [oxime, yellow prisms, m. 255° (from EtOH-dioxane)]; m-O2NC6H4, yellow prisms, m. 255° (from EtOH-dioxane)]; m-O2NC6H4, yellow prisms, m. 212° (from EtOH-dioxane); m-McG6H4, m. 178° (from EtOH); p-McGH4, m. 168° (from EtOH); p-C106H4, prisms, m. 166° (from EtOH); m-C106H4, m. 234° (from dioxane); PhCH2, yellow needles, m. 155° (from EtOH); 2-pyridyl, m. 177° (from EtOH); 3-pyridyl, m. 178° (from EtOH); 4-pyridyl, m. 172° (from EtOH). 7474-08-0P, 4H-1,3-Benzothiazin-4-one, 2-phenyl-10961-67-9P, 4H-1,3-Benzothiazin-4-one, 2-pp-nitrophenyl) 106274-04-8P, 4H-1,3-Benzothiazin-4-one, 2-(p-nitrophenyl) 106274-04-8P, 4H-1,3-Benzothiazin-4-one, 2-(m-nitrophenyl) 107915-37-7P, 4H-1,3-Benzothiazin-4-on

67433-04-9 CAPLUS 4H-1,3-Benzothiazin-4-one, 2-(phenylmethyl)- (CA INDEX NAME)

2-[m-chiotophenyi]- 10/31-37-7/, 4m-i, 3-benzothiazin-4-one, 2-2-p-tolyi- 10/317-93-1P, 4H-1,3-Benzothiazin-4-one, 2-RL: PREP (Preparation) (preparation of) 7474-08-0 CAPLUS 4H-1,3-Benzothiazin-4-one, 2-phenyi- (CA INDEX NAME)

L4 ANSWER 43 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

100961-67-9 CAPLUS

4H-1,3-Benzothiazin-4-one, 2-[p-(methylsulfonyl)phenyl]- (6CI) (CA INDEX

106274-04-8 CAPLUS 4H-1,3-Benzothiazin-4-one, 2-(4-nitrophenyl)- (CA INDEX NAME)

106274-94-6 CAPLUS
4H-1,3-Benzothiazin-4-one, 2-(m-nitrophenyl)- (6CI) (CA INDEX NAME)

106782-45-0 CAPLUS 4H-1,3-Benzothiazin-4-one, 2-(p-chlorophenyl)- (6CI) (CA INDEX NAME)

L4 ANSWER 44 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1957:99142 CAPLUS
DOCUMENT NUMBER: 51:99142
ORIGINAL REFERENCE NO.: 51:17927e-g
TITLE: Preparation and structure of some chloro derivatives of the phenothiazine and some derivatives of dichlorophenothiazine and some derivatives
AUTHOR(S): Antonov, D. Simov
SOURCE: Doklady Bolgarskoi Akademii Nauk (1956), 9(No. 4), 57-60
CODEN: DBANAD; ISSN: 0366-8681
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. C.A. 49, 5442c. 2,7-Diaminophenothiazine dioxide (I) (2,2 g.)
dissolved in 60 ml. H20 containing 3 ml. HCl, 60 ml. concentrated HCl
(37°)

added, and 7 ml. 10% solution NaNO2 dropwise added, the solution heated

50°, cuprous chloride catalyst (from 2.5 g. copper sulfate) added in one batch gave 1.06 g. 2,7-dichlorophenothiazine dioxide (II), m. 301-2°. II is identical with dichlorophenothiazine dioxide obtained from dichlorophenothiazine oxide. The position of the two chlorine atoms is thereby established.
7474-08-09, 48-1,3-Benzothiazin-4-one, 2-phenyl-RL: PREP (Preparation)
(preparation of)
7474-08-0 CAPLUS

(CA INDEX NAME)
7474-08-0 CAPLUS
4H-1,3-Benzothiazin-4-one, 2-phenyl- (CA INDEX NAME)

ANSWER 43 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

106782-86-9 CAPLUS 4H-1,3-Benzothiazin-4-one, 2-(m-chlorophenyl)- (6CI) (CA INDEX NAME)

107915-37-7 CAPLUS 4H-1,3-Benzothiazin-4-one, 2-(p-toly1)- (6CI) (CA INDEX NAME)

107917-93-1 CAPLUS 4H-1,3-Benzothiazin-4-one, 2-(m-toly1)- (6CI) (CA INDEX NAME)

L4 ANSWER 45 OF 45 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1955:84282 CAPLUS
DOCUMENT NUMBER: 49:84282
OXC COMPOUNDED OXC CAPPORATE SOURCE: Univ. Marburg/Lahn, Germany
SOURCE: Arch. Pharm. (1953), 286, 437-41
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
CTHER SOURCE(S): CASRACT 49:84282
AB of. C.A. 49, 8289a. S-Acetylthiosalicylamide (I) was prepared in low yield
by treating Na thiosalicylamide with AcCl in C6H6 (cf. Reissert and Manns,
C.A. 22, 4114) and in good yield from thiosalicylamide (II) and AcCl in C5H5N; S-propionylthiosalicylamide (III) was prepared in analogous manner.

manner.

Solns. of S-acylthiosalicylamides saturated with HCl, on addition of

Solns. of S-acylthiosalicylamides saturated with view of Solns. of S-acylthiosalicylamides saturated with view of toluene, distillation, and working up the residue yield the corresponding benzothiazine derivs. 4-0xo-2-phenyl-5,6-benzo-1,3-thiasine (IV), yellowish crystals, m. 122-3* (from absolute EroH or MeoBH, was prepared in 59% yield by passing HCl for several min. through 2.0 g. S-benzoylthiosalicylamide in 20 ml. xylene at 140°, raising the temperature slowly, and distilling slowly (60-75 min.) while passing a little HCl

little HCI through the solution, removing traces of solvent from the oily residue in vacuo, dissolving it in 20 ml. C6H6, removing unreacted amide with N

vacuo, dissolving it in 20 ml. C6H6, removing unreacted amide with N / washing with H2O, dtying over CaCl2, and removing C6H6. IV.HCl is not stable. I, colorless prisms, m. 148° (from EtOAc), was prepared in 88° yield by adding 5.1 g. AcCl drop by drop to 10.0 g. II in 25 ml. anhydrous C5H5N while stirring, letting stand 30 min. at -15°, adding 80 ml. Et2O, triturating with 50 ml. dilute H2SO4 at 0°, filtering, washing with H2O, and drying. N.S.-Diacetylthiosalicylamide, colorless needles, m. 74-5°, was prepared by refluxing I with excess Ac2O 5-6 hrs. 4-Oxo-2-methyl-5,6-benzo-1,3-thiazine-HCl, m. about 140° (decomposition), was prepared in 748 yield from I like IV, free base m. about 190° (decomposition), sintering 180°) (from C6H6.). III, colorless needles, m. 107-8°, was prepared like I in 96% yield. 4-Oxo-2-ethyl-5,6-benzo-1,3-thiazine-HCl, m.p. not given, was prepared in 41% yield like IV, free base, yellow powder, m. 50-60°. 7474-08-0P, 4H-1,3-Benzothiazin-4-one, 2-methyl-, hydrochloride 854067-02-0P, 4H-1,3-Benzothiazin-4-one, 2-methyl-, hydrochloride 854067-02-0P, 4H-1,3-Benzothiazin-4-one, 2-ethyl-, hydrochloride 854067-02-0P, 4H-3-Benzothiazin-4-one, 2-ethyl-, hydrochloride 854067-02-0P, 4H-3-Benzothiazin-4-one, 2-ethyl-, hydrochloride 854067-02-0P, 4H-3-Benzothiazin-4-one, 2-ethyl-, hydrochloride 87407-08-0 CAPLUS 4H-1,3-Benzothiazin-4-one, 2-ethyl-, hydrochloride 87474-08-0 CAPLUS

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RN 854066-98-1 CAPLUS CN 4H-1,3-Benzothiazin-4-one, 2-methyl-, hydrochloride (5CI) (CA INDEX NAME)

RN 854067-00-8 CAPLUS CN 4H-1,3-Benzothiazin-4-one, 2-methyl- (CA INDEX NAME)

854067-02-0 CAPLUS 4H-1,3-Benzothiazin-4-one, 2-ethyl-, hydrochloride (5CI) (CA INDEX NAME)

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RN 854067-04-2 CAPLUS
CN 4H-1,3-Benzothiazin-4-one, 2-ethyl- (CA INDEX NAME)

Habte 2/13/2008